



ARBEITSBERICHT NAB 25-04

THM-TH Abstraction of HLW Nearfield

April 2025

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

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KEYWORDS

Thermal-hydrological-mechanical processes, thermal hydrological modelling, abstraction, inverse modelling, effective parameter estimation, compressibility, uncertainty propagation analysis, iTOUGH2

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Abstract

The evolution of the nearfield around a disposal tunnel for high-level radioactive waste (HLW) depends on complex coupled thermal-hydrological-mechanical processes. However, the computationally expensive performance assessment (PA) calculations are preferably conducted using a simpler conceptual model that only explicitly accounts for thermal-hydrological (TH) processes. This simplification requires a THM-to-TH abstraction step. It is proposed that THM processes can approximately be represented by determining effective TH parameters. These effective parameters are estimated by the inversion of data reflecting THM processes using a TH model. The validity of this process is examined by generating synthetic THM data – calculated by a THM simulation of a two-dimensional cross section of a HLW disposal tunnel – and inverting the synthetic THM data using a TH model of the same cross section.

The THM numerical model was developed using Code_Aster (EDF 2024), which simulates the coupled non-isothermal two-phase flow and hydro-mechanical phenomena associated with repository-induced effects in the nearfield of an SF/HLW repository. Estimation of the effective parameters is performed using the iTOUGH2 simulation-optimization framework (Finsterle et al. 2017), which provides inverse modelling capabilities for TOUGH2 (Pruess et al. 2012), a code that simulates multiphase, multicomponent, non-isothermal fluid flow in porous media.

The primary goal of the modelling study was to obtain an abstracted iTOUGH2 TH model that could effectively predict the maximum pressures in the Opalinus Clay. The impact of potential sources of uncertainty in the iTOUGH2 model on predictions of interest was evaluated through Monte Carlo simulations with Latin Hypercube Sampling. It was demonstrated that the impact of overall model uncertainty, such as small amounts of uncertainty in the permeability of geological formations, affects prediction uncertainty far more than the small amount of uncertainty introduced from the model abstraction step.

Another important achievement was, that estimating effective pore expansivity and pore compressibility coefficients (a) from high-fidelity THM models, or (b) directly from site characterisation data (preferred) is an acceptable THM-to-TH abstraction approach. Uncertainties in the predicted maximum overpressures caused by uncertainties in the estimated, effective pore expansivity and pore compressibility coefficients are acceptable; the influence of residual errors from the model abstraction process on predictions of interest (e.g., maximum overpressures) is considerably smaller than the influence of random and systematic errors caused by the uncertainties on other parameters and model assumptions.

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List of Acronyms

Code Aster	Analysis of Structures and Thermomechanics for Studies & Research - Multi-Physics Finite Element Code
EBS	Engineered Barrier System
EDZ	Excavation damage zone
HLW	High-level waste
OPA	Opalinus Clay
PA	Performance assessment
SF	Spent fuel
TH	Thermo-hydrological
THM	Thermo-hydro-mechanical
TOUGH, iTOUGH2	Transport Of Unsaturated Groundwater and Heat - Suite of Simulators for Nonisothermal Multiphase Flow and Transport in Fractured Porous Media

1 Introduction

1.1 Background

The evolution of the nearfield around a disposal tunnel for high-level radioactive waste (HLW) depends on complex coupled thermal-hydrological-mechanical processes. However, the computationally expensive performance assessment (PA) calculations are preferably conducted using a simpler conceptual model that only explicitly accounts for thermal-hydrological (TH) processes. This simplification requires a THM-to-TH abstraction step. It is proposed that THM processes can approximately be represented by determining effective TH parameters. These effective parameters are estimated by the inversion of data reflecting THM processes using a TH model. The validity of this process is examined by generating synthetic THM data – calculated by a THM simulation of a two-dimensional cross section of a HLW disposal tunnel (see Fig. 1-1) – and inverting the synthetic THM data using a TH model of the same cross section.

Estimation of the effective parameters is performed using the iTOUGH2 simulation-optimization framework (Finsterle et al. 2017), which provides inverse modelling capabilities for TOUGH2 (Pruess et al. 2012), a code that simulates multiphase, multicomponent, non-isothermal fluid flow in porous media. While TOUGH2 serves as the TH simulator in this study, it is worth noting that the TOUGH family of codes also includes versions with coupled geomechanical simulation capabilities (e.g., Rutqvist et al. 2002).

The THM numerical model was developed using Code_Aster (EDF 2024), which simulates the coupled non-isothermal two-phase flow and hydro-mechanical phenomena associated with repository-induced effects in the nearfield of an SF/HLW repository. It is a two-dimensional (2-D) plain-strain finite element model, representing the stack of geological formations at the location of the SF/HLW component model in Nördlich Lägern. It comprises the 22 sequences of Mesozoic formations from the Permocarbon to the Malm, as shown in Fig. 1-1. The model represents the latest design for a repository at the Nördlich Lägern site. Additional details of the THM model, the geological setting and repository characteristics are given in Appendix A.

Finally, the evolution of pore pressures and temperatures as calculated by the abstracted TH model based on effective parameters are processed to estimate the total stress evolution using an approximate semi-analytical solution. While this post-processing step does not account for the feedback between non-elastic, non-volumetric, anisotropic stress-strain relations and hydrological properties and consequential flow behaviour, it allows for an approximate estimation of the stress state within the bentonite backfill and the potential occurrence of large deformations, failures, or impacts on the adjacent host rock.

1.2 Objectives

The main objective of this study is to evaluate the ability of an abstracted TH model to reproduce and/or predict the behaviour of an HLW nearfield representative of a disposal tunnel based on the latest design for a repository at the Nördlich Lägern site. The abstraction process is based on the estimation of effective parameters for the engineered barrier system (EBS) and surrounding geosphere using inverse modelling of synthetic data generated by a THM model of the HLW tunnel.

The outline of this report is as follows. In Section 2, the overall model setup is described, including the conceptual model, the computational grid, property assignment, and the steps that are used to simulate the evolution of conditions in the repository before and during emplacement of the waste canister (i.e., steady-state initialization, the excavation and ventilation phase, and the heating phase, along with corresponding changes to initial and boundary conditions, and material assignments). In Section 3, the development of the Code_Aster and iTOUGH2 models is described,

including a comparison of the simulation output for the models, with some differences noted among the initial iTOUGH2 simulation, and the TH and THM versions of the Code_Aster simulations. The iTOUGH2 model serves as the basis for a sensitivity analysis that is shown in Section 4, in which the sensitivity of the simulation output to various input parameters is examined, helping to determine which parameters and data sets are suitable to include in model calibration. The model calibration results are given in Section 5. The calibrated model is then used in Section 6 to evaluate (a) the relative impact that subsets of effective parameters have on model predictions; (b) prediction uncertainty due to the actual parameter uncertainty arising from the THM to TH abstraction process itself (i.e., parameter probability distributions are based on the effective TH parameters and their standard deviations estimated in model calibration), and some conservative variations that introduce additional uncertainty; and (c) prediction uncertainty that is not due to the model abstraction process but due to other sources of uncertainty in the conceptual model and the geological environment in which it is applied. Section 7 presents the post-processing step of analysing total stresses in response to swelling pressures and thermal expansion and contraction effects. Finally, Section 8 provides a summary and some conclusions.

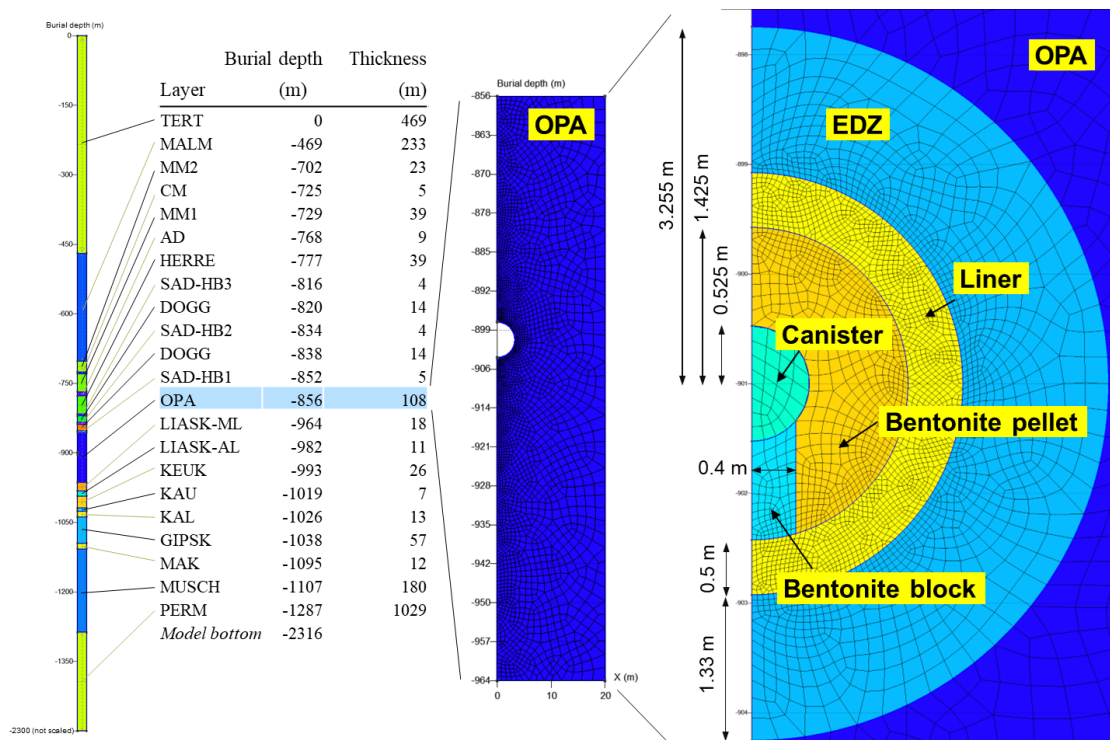


Fig. 1-1: Stratigraphic layers in the SF/HLW model for Nördlich Lägern and discretization for Code_Aster
(see Appendix A)

2 Model setup

2.1 Conceptual model

The conceptual model includes features and processes that may potentially affect the thermal and hydrological conditions within the EBS and surrounding geosphere. The following mechanisms are included in the model:

- Two-phase (gas and liquid) flow of two components (water and air) through porous media based on a multi-phase extension of Darcy's law
- Vaporization and condensation of water; degassing and dissolution of air in the liquid and gas phases
- Heat transport by conduction, convection, and multi-phase diffusion; latent heat effects
- Gravitational, viscous, and capillary forces
- Phase interference (relative permeability) effects
- Pressure-dependent porosity changes based on (1) an implementation of the Bishop formulation (Nuth & Laloui 2008, Pereira et al. 2010) in which the change in effective pressure is given by the aqueous-phase saturation multiplied by the change in capillary pressure, and (2) a standard linear formulation for pore compressibility (Pruess et al. 2012)
- Temperature-dependent porosity changes based on a linear thermal pore expansion coefficient (Pruess et al. 2012)

2.2 Computational grid

The computation grid, shown in Fig. 2-1, comprises a two-dimensional cross section of an HLW disposal tunnel and the surrounding geological formations and has the following characteristics:

- Only half of the tunnel and surrounding formations needs to be discretized due to a vertical plane of symmetry.
- The grid has a total width of 20 m (X direction), a thickness of 1 m (Y direction), and it extends from the ground surface to a burial depth of -2,316 m (Z direction).
- It is an unstructured grid containing 2D radial components, and 1D and 2D Cartesian components, with a total of 1,455 grid blocks and 2,821 connections.
- The radial component has (a) its origin at the centre of the waste canister at $X = 0$ m, $Z = -910$ m; (b) radial spacing of 0.1 m to 0.5 m, with a maximum radius of approximately 4.5 m; and (c) angular spacing of 5 to 15 degrees. It covers the region with the tunnel materials (liner, waste canister, and bentonite buffer), and the EDZ, and it extends ~1 m radially into the host rock surrounding the EDZ.
- A Cartesian component, with a grid spacing of 0.5 m, is embedded within the radial component of the grid for the purpose of discretizing the bentonite pedestal in such a way as to allow for the accurate placement of the (curved) interfaces it shares with the canister and the liner (at a radius of 0.525 m and 1.525 m, respectively), and the (vertical) interface it shares with the bentonite buffer (at $X = 0.4$ m).
- Surrounding the tunnel region (radii > 1.425 m), Cartesian components with increasingly coarse levels of discretization are used, as follows: (a) the first region surrounds the tunnel ($0 < X < 10$ m, $-920 < Z < -900$ m) and uses 1 m spacing, and is surrounded by (b) a second Cartesian region with spacing of 2 m that spans the entire horizontal extent of the grid

($0 < X < 20$ m) and extends roughly ± 50 m in the vertical direction ($-962 < Z < -858$), which transitions to (c) upper and lower 2-D regions (for $-1,000 < Z < -850$, and $-1,000 < Z < -850$), with spacing of 5 m, and then transitions to (d) upper and lower 1-D components that extend to the respective upper and lower model boundaries, with a maximum grid spacing of 50 m.

- The grid nodes are carefully placed to position observation locations and interfaces between formations and tunnel materials such that they are consistent with the Code_Aster THM grid.

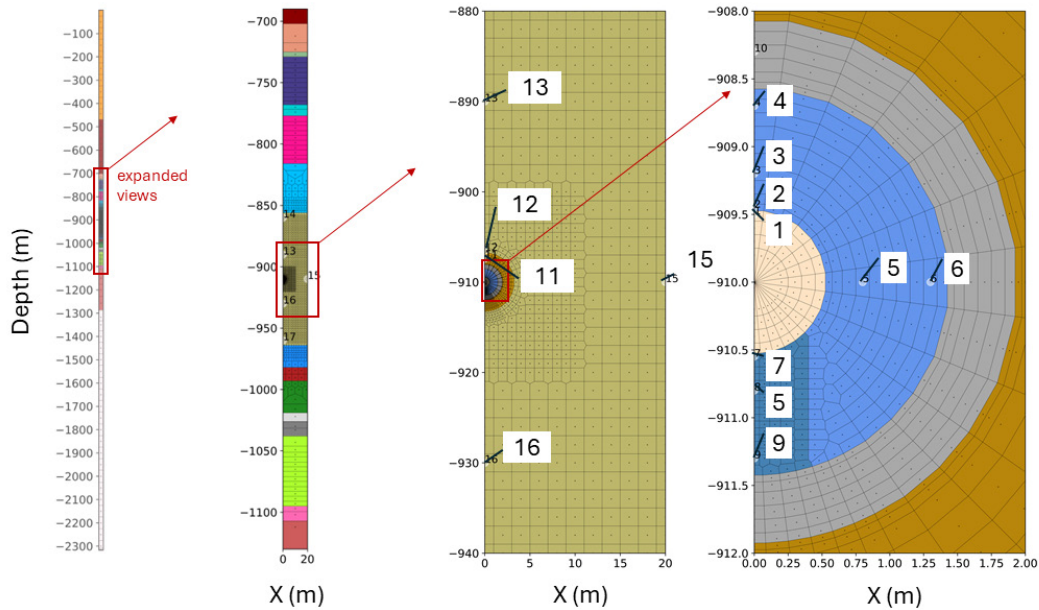


Fig. 2-1: Computational grid for iTOUGH2 TH model

2.3 Property assignment

Unless otherwise noted, the thermal and hydrological properties of the iTOUGH2 TH models are the same as those specified in the Code_Aster model (see Tab. A-1), with some exceptions (see Tab. 2-1). The pore compressibility values used in the comparison of the TH version of the Code_Aster model with the initial iTOUGH2 model in Section 3 are shown in the second column of Tab. 2-1 for reference. The pore compressibility values corresponding to the initial guesses and estimated values for the THM-TH inversion of Section 5.3.1 are shown in columns 3 and 4, respectively, in Tab. 2-1. Similarly, the pore expansivity values corresponding to the initial guesses and estimated values for the THM-TH inversion of Section 5.3.1 are shown in columns 5 and 6, respectively.

Note that isotropic permeability is used in this study, in part to avoid complications that arise when implementing anisotropy using an unstructured TOUGH2 numerical grid. In addition, the van Genuchten model (Luckner et al. 1989) is used to describe the relative permeability and capillary pressure as a function of liquid saturation, based on parameters given in Tab. A-1.

Tab. 2-1: Pore compressibility (c_p) and pore expansivity (Exp) parameters in TH models

Parameter	c_p (Pa ⁻¹)	c_p (Pa ⁻¹)	c_p^1 (Pa ⁻¹)	Exp (Pa ⁻¹)	Exp ² (Pa ⁻¹)
Description (→)	Section 3.3: iTOUGH2 & Code_Aster TH Comparison	Section 5.3.1: THM-TH Inversion (initial)	Section 5.3.1: THM-TH Inversion (final)	Section 5.3.1: THM-TH Inversion (initial)	Section 5.3.1: THM-TH Inversion (final)
Material (↓)					
TERT	1.67E-09	1.333E-09	1.333E-09	1.70E-05	1.70E-05
MALM	1.67E-09	1.333E-09	1.333E-09	1.70E-05	1.70E-05
MM2	2.38E-09	1.905E-09	1.905E-09	1.70E-05	1.70E-05
CM	5.00E-09	4.000E-09	4.000E-09	1.70E-05	1.70E-05
MM1	2.03E-09	1.622E-09	1.622E-09	1.70E-05	1.70E-05
AD	1.25E-09	5.000E-10	5.000E-10	1.70E-05	1.70E-05
HERRE	5.77E-09	4.615E-09	4.615E-09	1.70E-05	1.70E-05
SAD-HB3	1.22E-09	1.402E-09	8.889E-10	1.70E-05	1.70E-05
DOGG					
SAD-HB2					
DOGG					
SAD-HB1					
OPA (HOST)	2.10E-09	1.714E-09	7.230E-10	1.70E-05	1.438E-04
LIASK-ML	2.00E-09	1.600E-09	1.373E-09	1.70E-05	1.70E-05
LIASK-AL	1.81E-09	1.446E-09	1.446E-09	1.70E-05	1.70E-05
KEUK	1.39E-09	9.298E-10	9.298E-10	1.70E-05	1.70E-05
KAU	1.73E-09	1.395E-09	1.395E-09	1.70E-05	1.70E-05
KAL	1.24E-09	1.043E-09	1.043E-09	1.70E-05	1.70E-05
GIPSK	1.65E-09	5.416E-09	5.416E-09	1.70E-05	1.70E-05
MAK	9.00E-09	9.231E-09	9.231E-09	1.70E-05	1.70E-05
MUSCH	1.25E-09	1.000E-09	1.000E-09	1.70E-05	1.70E-05
PERM	1.25E-09	1.000E-09	1.000E-09	1.70E-05	1.70E-05
EDZ	1.70E-09	4.444E-09	4.289E-10	1.70E-05	1.70E-05
LINER	7.00E-10	6.900E-10	6.900E-10	1.50E-05	1.50E-05
CANIS	1.000E-10	6.000E-09	6.000E-09	1.20E-05	1.20E-05
BLOCK	3.00E-09	1.000E-10	1.000E-10	2.50E-05	2.50E-05
PELLET	3.00E-09	1.000E-10	1.000E-10	2.50E-05	2.50E-05

¹ Pore compressibility values derived from elastic data (unshaded cells) or log values estimated (shaded cells) by inversion.

² Pore expansivity fixed (unshaded cells) or log value estimated (shaded cell) by inversion.

2.4 Description of simulation steps and corresponding initial conditions, boundary conditions, and material assignments

The repository-induced thermal and hydrologic processes occurring in the nearfield of an SF/HLW repository are calculated in a series of simulation steps for which the respective initial and boundary conditions and emplacement of materials are specified as follows.

1. Initial equilibration phase to simulate steady-state conditions: Calculate approximate hydrostatic pressure and temperature profiles under fully liquid-saturated conditions assuming (a) the pressure at the ground surface is 0.1 MPa (1 atm); (b) all other faces of the model domain have no-flow boundaries; and (c) the initial temperature gradient is 0.043 °C/m, with a 10 °C offset at the surface (reflecting the near-surface groundwater temperature) and with the temperature at the lower boundary fixed to its corresponding initial value. The simulation time for this phase is 2 million years.
2. Two-week excavation/pre-ventilation phase to simulate the effect of tunnel excavation (namely reduced pressure) as the excavation nears but has not yet reached the boundary of the model domain: The hydrostatic pressure and temperature profiles calculated in Step 1 serve as the initial conditions in this simulation phase, with the following additional specifications: (a) as in Step 1, fix the pressure and temperature at the top model boundary, and the temperature at the lower boundary to the respective previously specified values; (b) fix the pressure at the lower boundary (at a depth of -2316 m) to the hydrostatic value calculated in Step 1 (to be fixed for the remaining simulation phases); (c) continue using no-flow boundary conditions at the two vertical faces of the model domain (to remain in place for the remaining simulation phases); (d) in the model region where the tunnel will be emplaced, fix the pressure to 0.1 MPa and the capillary pressure to 0. Set the pore compressibility and pore expansivity for all materials to 0, to be consistent with the Code_Aster simulation.
3. Two-year ventilation phase after the tunnel is excavated and opened to the atmosphere and the liner is instantaneously emplaced: Starting with the hydrostatic pressure and temperature distributions calculated in Step 2 as initial conditions, make the following additions: (a) the region contained within the liner – which will contain the pedestal and bentonite buffer, and the canister – is modelled as an open cavity that is connected to the atmosphere by fixing the pressure to 0.1 MPa, the relative humidity to ~60%, and the temperature to 28 °C.
4. Post-closure phase after the bentonite and canister materials are emplaced and the tunnel is instantaneously closed to the atmosphere, and a time-dependent heat source is applied in the canister: Starting with the hydrostatic pressure and temperature distributions calculated in Step 3 as initial conditions, make the following additions: (a) the canister, pedestal, and bentonite buffer are added with initial gas saturations of 0.5, 0.5, and 0.8, respectively, and (b) a time-dependent heat source is applied to the HLW canister (see Fig. 2-2). The simulation time for this phase is 100,000 years.

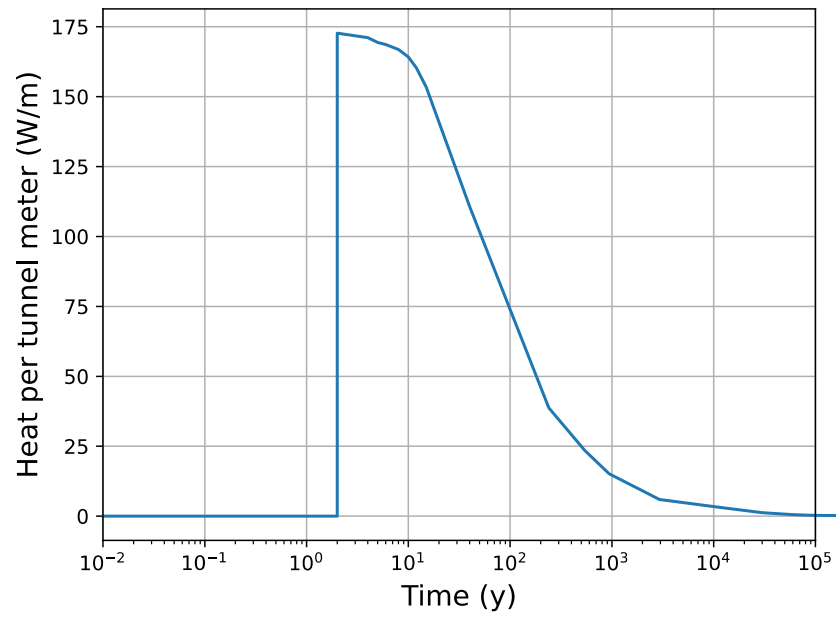


Fig. 2-2: Time-dependent heat source applied to the HLW canister

3 Development of Code_Aster and iTOUGH2 models

3.1 Simulation output

The evolving system state, including pressure, liquid saturation, temperature, and porosity – calculated at each grid point and for each time step – is extracted at 17 locations (“control points”) (1) to generate “synthetic data” with the Code_Aster THM model, and (2) to simulate corresponding iTOUGH2 performance measures as part of the sensitivity analyses, model calibration and prediction uncertainty analyses. The control points are placed at strategic locations (see Fig. 2-1 and Fig. 3-1) with the expectation that they provide informative data for model calibration, leading to accurate parameter estimates and model predictions. Of particular interest is prediction of the maximum pressures in the host rock (Opalinus Clay), especially at P13 and P15, which are positioned 20 m above and to the side of (in the lateral direction) the waste canister, respectively.

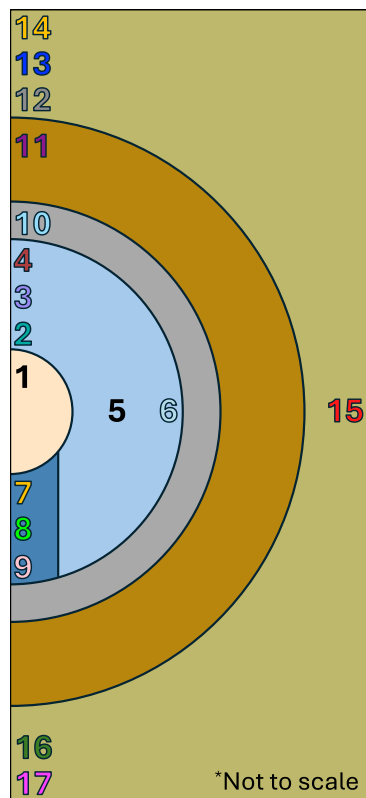


Fig. 3-1: Schematic depicting relative positions of control points
(see Fig. 2-1 for dimensions)

3.2 Consistency between models

Efforts were made to identify and minimize non-THM-related discrepancies between the Code_Aster and iTOUGH2 models. The goal was to develop an initial iTOUGH2 model – to be used as the basis for model calibration – that is as consistent as possible with a corresponding TH version of the Code_Aster model, insuring that (1) the same systems are being simulated in each model (consistent boundary conditions, rock properties, simulation steps, etc.), and (2) the only differences that arise between the THM version of the Code_Aster model and the iTOUGH2 TH model using effective parameters (pore expansivity, and pore compressibility for a limited number of materials); the effective parameters are estimated subsequently in model calibration.

As part of this process, a TH-only version of the Code_Aster model (“run03f”) – which includes thermal-hydrological processes but not mechanical deformation processes – was developed for comparison with the initial iTOUGH2 model to help identify initial discrepancies between the models while ruling out mechanical effects as a cause. Some slight differences in the simulation output that were initially observed were traced back to differences in implementation of the conceptual model and the numerical model (e.g., specification of heat source and boundary conditions, residual gas saturation, details of the porosity function, discretization of tunnel materials, times required to obtain consistent near-steady-state distributions for equilibration phase, and other details related to the initialization of different simulation phases). After several iterations of coordinated model refinement, the simulation output was judged to be sufficiently similar for the purposes of this study (i.e., prediction of pressures in the host rock). While some differences remain, as noted in Section 3.3, further investigation of their causes will be left for future studies.

3.3 Comparison of Code_Aster TH and initial iTOUGH2 simulations

The pressures, temperatures, liquid saturations, and porosity values simulated as a function of time by the TH version of the Code_Aster model and the initial iTOUGH2 model are discussed next. For this case, both models use the same TH input parameters (see Tab. A-1 and Tab. 2-1), which should theoretically result in the same simulated properties; however, the results may differ slightly nonetheless, as Code_Aster and iTOUGH2 each make different underlying assumptions and approximations for the simulation of multiphase flow and transport (e.g., handling of flow in the gas phase) and may have different implementations of physical properties (e.g., relative permeability, capillary pressure).

3.3.1 Pressure

The heat generated in the waste canister, followed by an increase in temperature and thermal expansion of the surrounding pore fluid and materials, results in a complex pressure response, as shown in Fig. 3-2. For the two years before heating begins, the repository tunnel is considered open to the atmosphere (accomplished by fixing the pressure in the liner to atmospheric conditions). As a result, the pressures decrease above the canister in the EDZ at P11 and just above that in the host rock at P12. The pressures at the remaining control points remain mostly steady in this period. After the instantaneous installation of the bentonite and canister materials and the onset of heating at 2 years, the pressures increase notably at the distant control points in the surrounding host rock, with maximum values occurring at approximately 100 years (P13, P15, P16) and 600 years (P14 and P17). At later times, the pressure response becomes further complicated by the superposition of various pressure wave reflections (e.g., from underlying geological formations, the vertical boundary on the right side of the model, and the lower boundary of the model).

The pressures simulated by Code_Aster and iTOUGH2 match reasonably well, although the iTOUGH2 model calculates maximum pressures that are higher (on the order of 1 MPa) than those calculated by Code_Aster, and the simulated pressures diverge somewhat at later times (after ~1,000 years). The steady-state pressures at early times are in good agreement.

Efforts have been made to identify the reasons behind these residual mismatches in pressures – and to modify the models accordingly to make them more consistent – but they have been unsuccessful so far; further consideration of the issue is left for future studies. Regardless, the model calibration procedure considered in this study in which the iTOUGH2 model will be calibrated based on synthetic data generated by a Code_Aster simulation (specifically, using the THM version of the Code_Aster model, as will be discussed below), will allow any such mismatch in pressures to be overcome, providing a calibrated TH model that is capable of accurately predicting the processes of interest, including the pressures in the host rock.

The abstraction consists of estimating effective parameters by matching the pressure evolution calculated by the TH model to that obtained by the THM model. Because there are differences in the pressures calculated by the two models even without accounting for mechanical processes, the abstraction is not exclusively focused on addressing mechanical effects, but it also needs to compensate for non-mechanical differences in the two model implementations of two-phase flow. As a consequence, the differences between the calibrated, effective parameters and the corresponding, more physical properties used in the high-fidelity THM model cannot solely be attributed to the abstraction of mechanical effects, but also contain contributions from the inherent discrepancies between the two models' representation of TH processes.

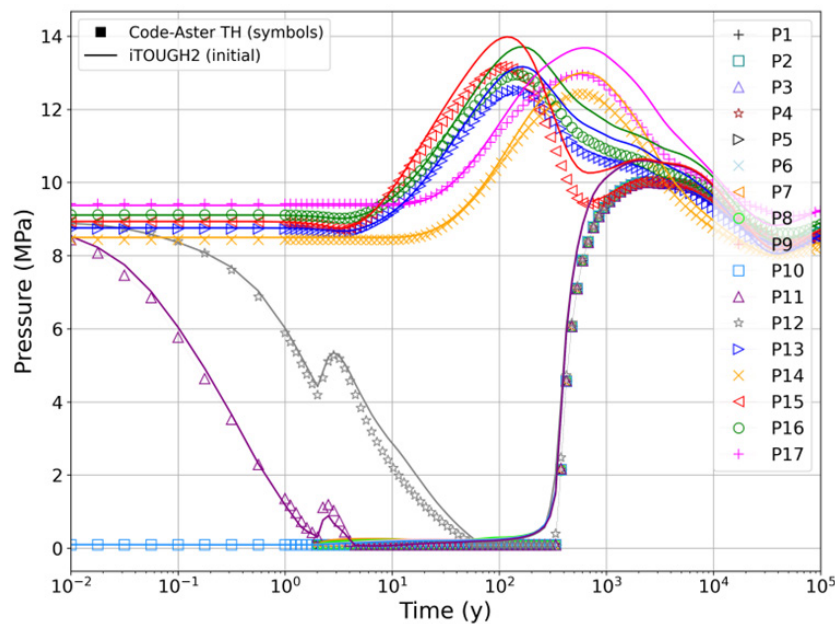


Fig. 3-2: Pressures simulated with Code_Aster TH model and initial iTOUGH2 model

3.3.2 Temperature

The temperature response is shown in Fig. 3-3. In the first two years, after the tunnel is excavated but before the canister and bentonite materials are installed and assuming the ventilation system uses ambient rather than cooled air, the simulated temperatures are (1) constant at 28 °C in the concrete liner (P10), (2) declining above the liner in the EDZ at P11 and in the overlying host rock at P12 due to the presence of the tunnel, and (3) steady at the control points in the remaining geological formations surrounding the tunnel. After two years, the temperatures increase due to the heat from the waste canister, with a maximum temperature occurring between approximately 10 and 1,000 years.

Overall, the temperature match between models is very good, though there are some slight systematic deviations at several control points within the tunnel (P2, P3, P7, P8), most likely due to small differences in grid geometry (e.g., position of nodes or interfaces between grid blocks).

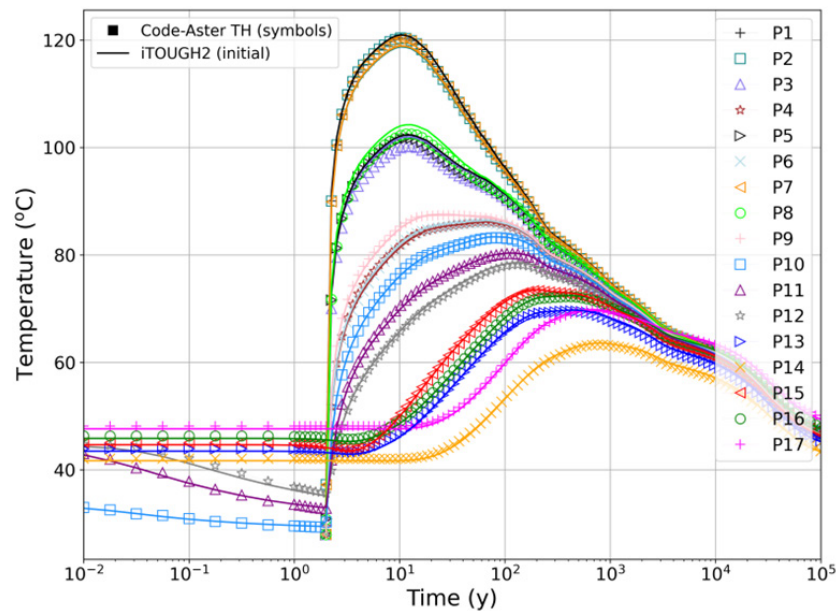


Fig. 3-3: Temperatures simulated with Code_Aster TH model and initial iTOUGH2 model

3.3.3 Saturation

The simulated saturation profiles are shown in Fig. 3-4. While the host rock at the distant control points P12 through P17 remains fully liquid saturated for the entire simulation, wetting and drying processes occur within the tunnel and the EDZ over a period of around 400 years, which is reflected in the saturation profiles at control points P1 through P11.

During the steady-state phase of the simulation, the entire region containing control points is fully liquid saturated. After the tunnel is excavated and the concrete liner is installed (i.e., during the ventilation phase), the open tunnel on the inside of the liner is open to the atmosphere, while the concrete liner itself is modelled as a porous material and is given an initial liquid saturation of 0.7. Then, over the course of the two-year ventilation phase, the saturation response at P10 (in the concrete liner directly above the waste canister) diverges for each model: saturation increases in the Code_Aster simulation (wetting behaviour) and decreases in the iTOUGH2 simulation

(drying behavior). The reason for the different wetting behavior between models during this period is unclear; however, by around 10 years, the saturation profiles become similar as the liner approaches its eventual liquid-saturated state.

Just above the concrete liner at P11 in the EDZ, partial desaturation begins to occur at around five years, which is predicted consistently for both models.

In the bentonite buffer material (with an initial saturation of 0.2 at 2 years), saturation at control points P2, P3, and P5 begins to increase, starting at around 20 or 40 years, in a consistent way for both the Code_Aster and iTOUGH2 models (note that the purple P3 line is almost directly behind the black P5 line.) By contrast, at control points P4 and P6, which are positioned closer to the liner, the wetting process is less consistent between models. Similarly, at control points P7 and P8 in the bentonite block (with an initial saturation of 0.5 at 2 years), the saturation increases consistently for both models at around 40 years, but at control point P9, which is closer to the liner material, wetting begins sooner in the iTOUGH2 model and there is a slight difference between models at early times. These inconsistencies are likely related to differences in the capillary pressure and relative permeability curves and the general treatment of two-phase flow processes.

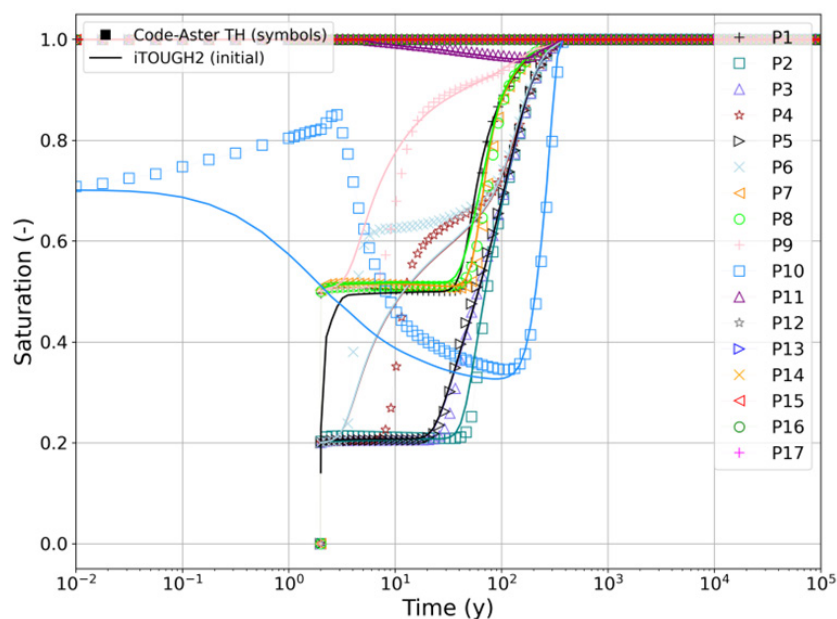


Fig. 3-4: Saturations simulated with Code_Aster TH model and initial iTOUGH2 model

3.3.4 Porosity

Simulated porosity values are shown for completeness (Fig. 3-5). Consistent trends are seen between the Code_Aster and initial iTOUGH2 models, but the largest differences between models occur in the bentonite materials (Fig. 3-5a). The sensitivity analysis presented in Section 4 will show that the simulated predictions of interest in this study, namely the pressure response, have low sensitivity to the absolute value of the initial porosity (see Fig. 4-1 and Fig. 4-2), but it is expected that sensitivity to the function that controls changes in porosity during the simulation period, which affect the pressure response, is significant.

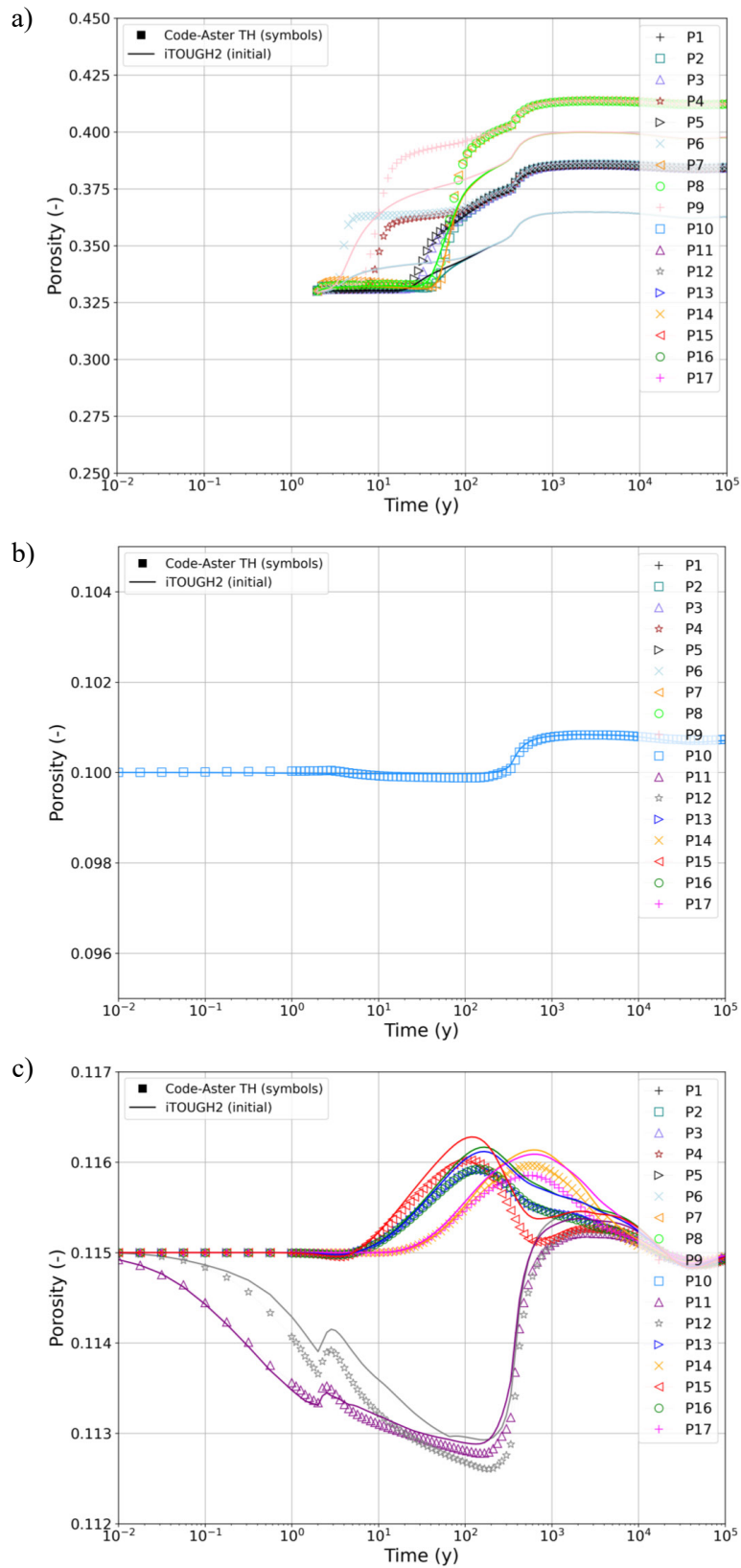


Fig. 3-5: Calculated porosity for Code_Aster TH model and initial iTOUGH2 model
 For controls points in (a) the bentonite materials (P2 through P9), (b) the liner (P10), and
 (c) EDZ (P11) and host rock (P12 through P17)

3.4 Comparison of Code_Aster THM and initial iTOUGH2 simulations

Simulated output from the THM version of the Code_Aster model (“run02d”), which is considered for the remainder of the study, is shown in Fig. 3-6 (pressures), Fig. 3-7 (temperatures), and Fig. 3-8 (saturation), as is the simulated output for the initial iTOUGH2 TH model.

As opposed to the comparison of the TH models in Section 3.3, in this case, the initial pore compressibility values used in the iTOUGH2 model are calculated from elastic data. These values are considered to be hypothetical and may be adjusted in model calibration (Tab. 2-1).

In particular, the preliminary pore compressibility values for the bentonite materials result in a surprisingly large misfit to the late-time pressures, temperatures and saturations simulated by the initial iTOUGH2 TH model, as shown in Fig. 3-6a, Fig. 3-7a, and Fig. 3-8a, respectively, casting doubt on their suitability for use in the model calibration.

Therefore, a second initial simulation was run with the pore compressibility values for the bentonite materials modified as follows: the log pore compressibility (units of $\log_{10}[1/\text{Pa}]$) for each was set to -10 instead of the values calculated based on the elastic data (-7.74 for the bentonite pedestal, and -7.53 for the bentonite buffer).

The resulting pressures, temperatures, and saturations, as shown in Fig. 3-6b, Fig. 3-7b, and Fig. 3-8b, result in a more reasonable starting point for model calibration.

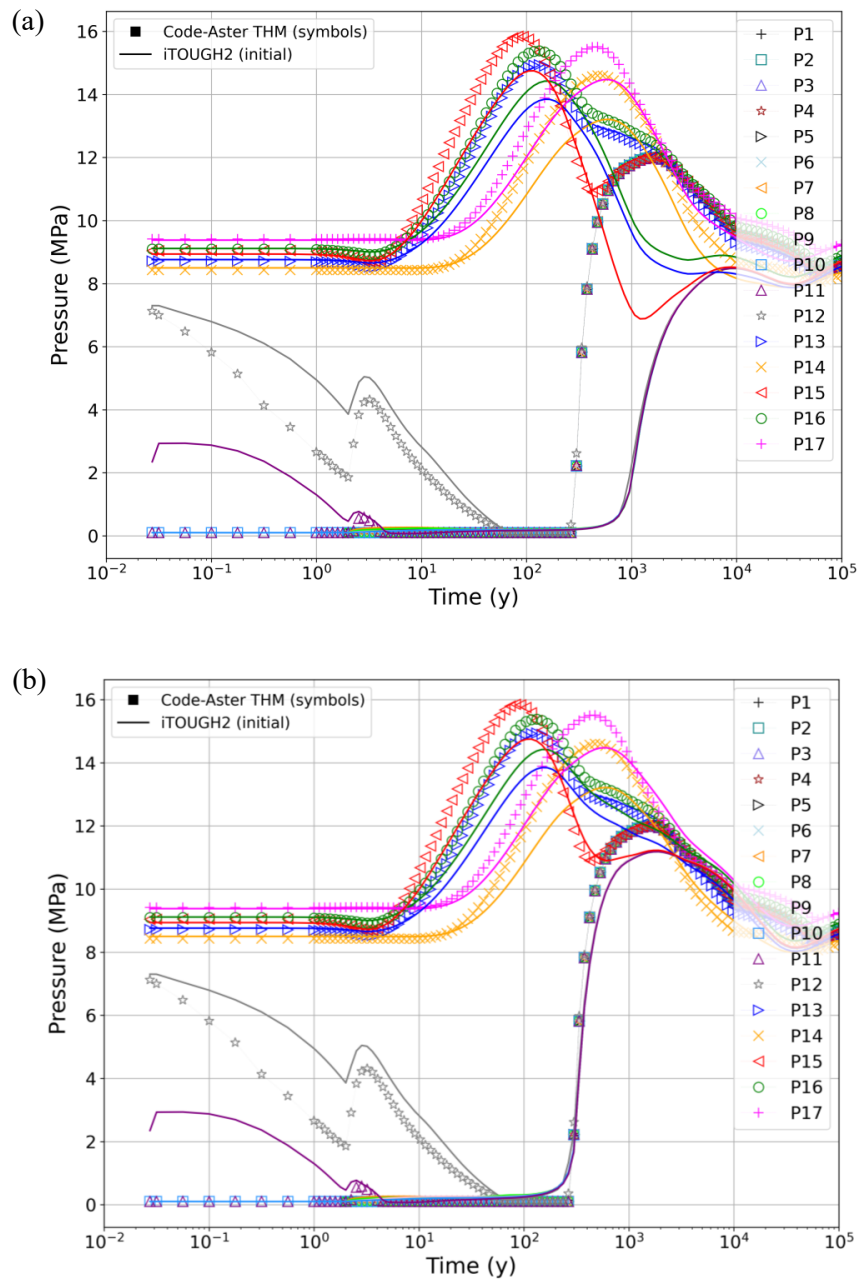


Fig. 3-6: Pressures simulated with the Code_Aster THM model compared with the initial iTOUGH2 model using log pore compressibility of bentonite materials

(a) same as Code_Aster model (-7.74 for pedestal, -7.53 for buffer), and (b) -10.0 for both

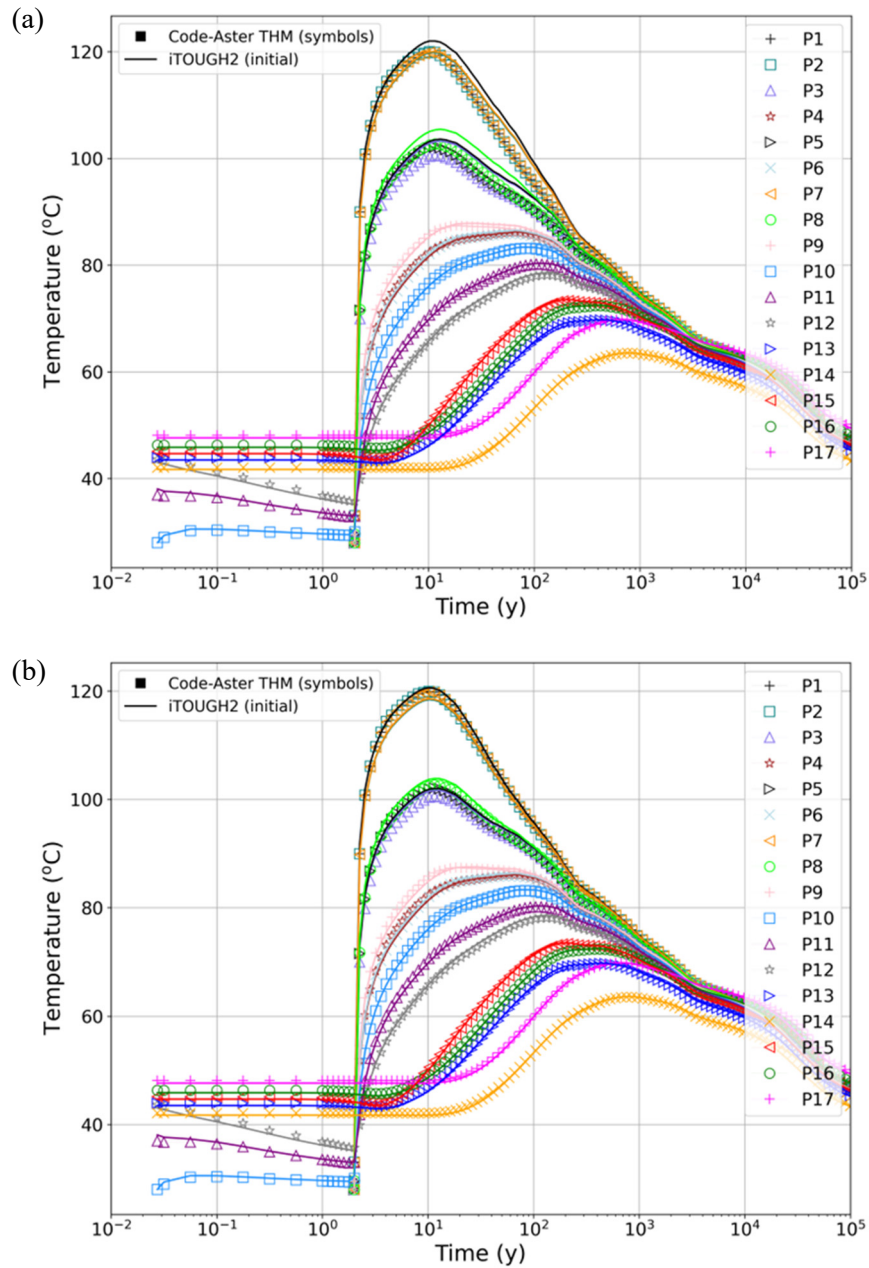


Fig. 3-7: Temperatures simulated with the Code_Aster THM model compared with the initial iTOUGH2 model using log pore compressibility of bentonite materials
 (a) same as Code_Aster model (-7.74 for pedesal, -7.53 for buffer), and (b) -10.0 for both

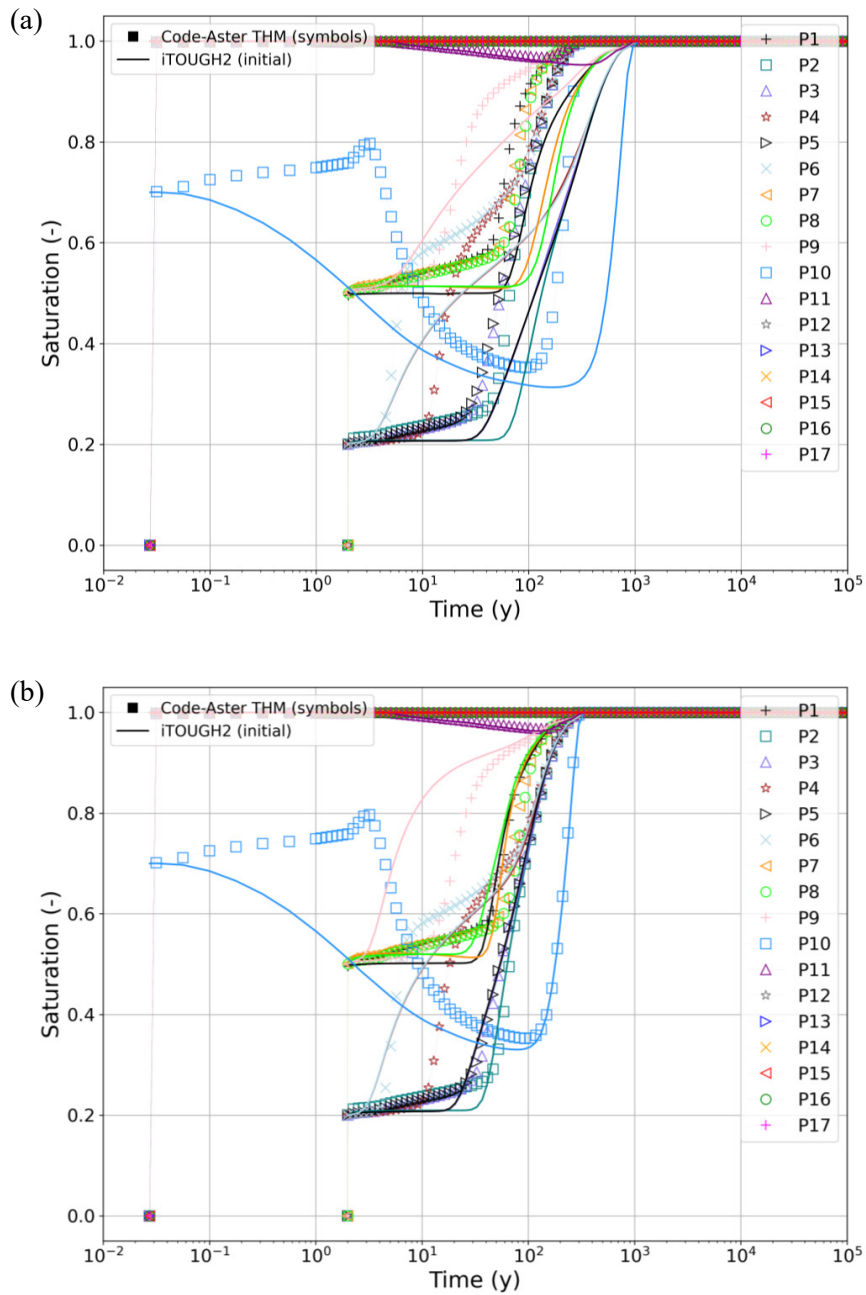


Fig. 3-8: Saturations simulated with the Code_Aster THM model compared with the initial iTOUGH2 model using log pore compressibility of bentonite materials

(a) same as Code_Aster model (-7.74 for pedestal, -7.53 for buffer), and (b) -10.0 for both

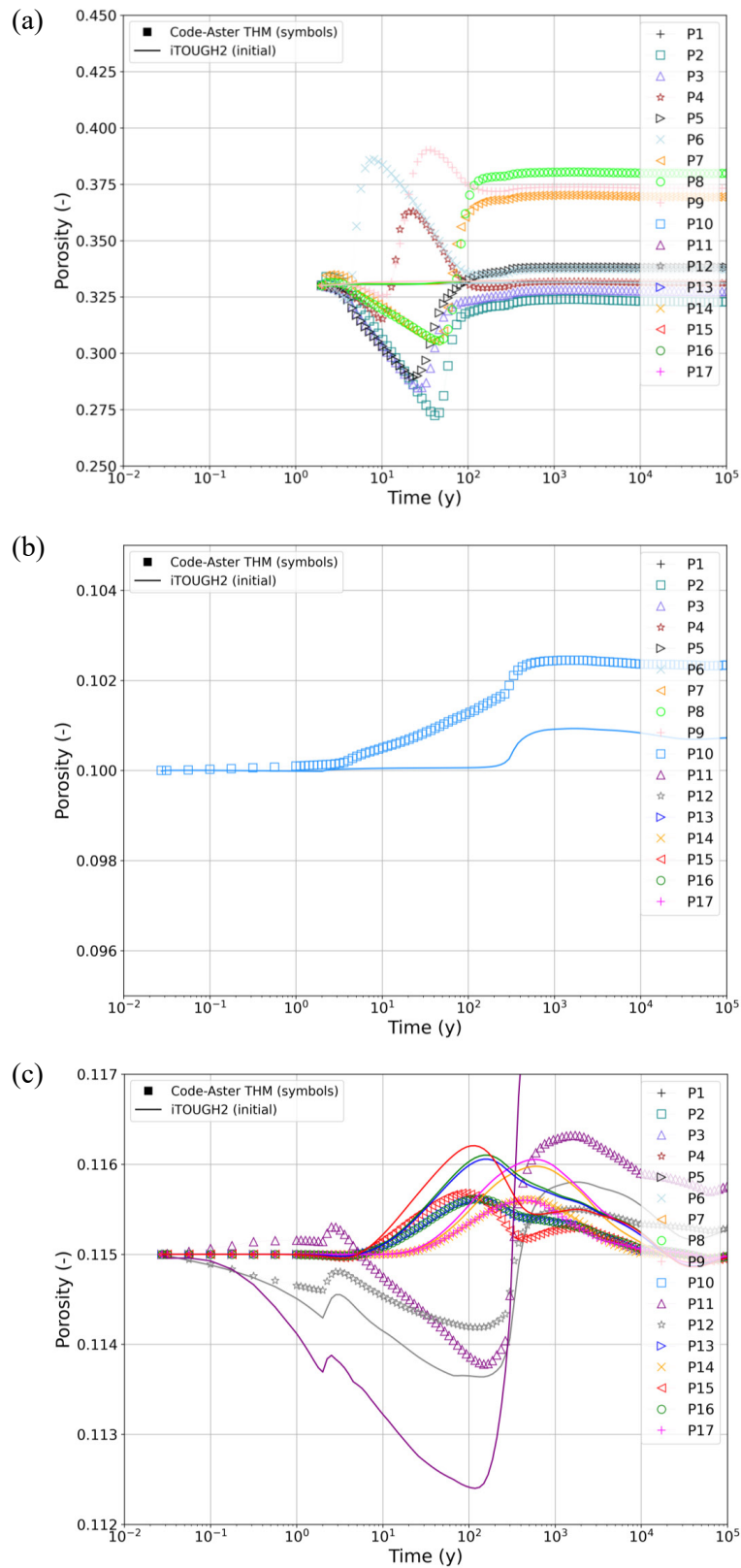


Fig. 3-9: Comparison of porosities simulated with the Code_Aster THM model and the initial iTOUGH2 model, with the latter using log pore compressibility of -10.0 for bentonite pedestal and buffer

4 Sensitivity analysis

4.1 Parameter selection and perturbation

Sensitivity analyses are performed in which parameters expected to influence the composite performance metrics are perturbed – one at a time – from reference values. The analysis focuses on parameters that specifically influence the pressures in the Opalinus Clay, as opposed to evolution of properties (e.g., liquid saturation) within the repository tunnel itself. Only a small subset of all potential parameters is selected, including pore expansivity, pore compressibility, permeability, porosity, and thermal conductivity for various materials. Relatively large perturbations are used to highlight the parameters' impact on the calculated performance metrics.

Two cases with different sets of reference values are considered, one based on a parameter set that is similar to the initial guesses to be used in model calibration (the only difference being in values of log pore compressibility of the bentonite buffer and pedestal, which are assumed to be -10.0 in model calibration), and one whose parameters are closer to values obtained in the model calibration discussed in Section 5. Tab. 4-1 and Tab. 4-2 show the selected parameters and their respective perturbations for both cases.

Tab. 4-1: Parameters examined by sensitivity analysis with reference values based on initial parameter guesses from Code_Aster THM model

Parameter	Material	Reference values	Perturb.
log pore expansivity ($\log_{10} [1/^\circ\text{C}]$)	Opalinus Clay: HOST, EDZ	-4.77, -4.77	1.0
log pore compressibility ($\log_{10} [1/\text{Pa}]$)	Opalinus Clay: HOST, EDZ Bentonite: PELL, BLOCK Formations: KEUK, AL, ML, DOGG, HERRE	-8.766, -8.352 -7.53, -7.74 -9.03, -8.84, -8.80, -8.85, -8.34	0.3
log permeability ($\log_{10} [\text{m}^2]$)	Opalinus Clay: HOST, EDZ Bentonite: PELL, BLOCK Formations: KEUK, AL, ML, DOGG, HERRE	-21.04, -20.04 -19.46, -21.04 -20.69, -20.74, -20.34, -20.65, -19.04	0.3
Porosity	Opalinus Clay (HOST): Bentonite (PELL, BLOCK):	0.115 0.33, 0.33	0.05
Thermal conductivity wet ($\text{W m}^{-1} \text{K}^{-1}$)	Opalinus Clay (HOST):	2.1	0.1
Thermal conductivity dry ($\text{W m}^{-1} \text{K}^{-1}$)	Opalinus Clay (HOST):	1.4	0.1

Tab. 4-2: Parameters examined by sensitivity analysis with reference values that are similar to the calibrated iTOUGH2 model

(red entries were varied in the process of model calibration, green entries were fixed to an appropriate value, black entries are the same as in the first case of Tab. 4-1; see Section 5)

Parameter	Material	Reference values	Perturb.
log pore expansivity ($\log_{10} [1/^{\circ}\text{C}]$)	Opalinus Clay: HOST, EDZ	-3.86, -3.86	1.0
log pore compressibility ($\log_{10} [1/\text{Pa}]$)	Opalinus Clay: HOST, EDZ Bentonite: PELL, BLOCK Formations: KEUK, AL, ML, DOGG, HERRE	-9.12, -10.80 -10.0, -10.0 -8.92, -8.99, -8.83, -9.06, -8.32	0.3
log permeability ($\log_{10} [\text{m}^2]$)	Opalinus Clay: HOST, EDZ Bentonite: PELL, BLOCK Formations: KEUK, AL, ML, DOGG, HERRE	-21.04, -20.04 -19.46, -21.04 -20.69, -20.74, -20.34, -20.65, -19.04	0.3
Porosity	Opalinus Clay (HOST): Bentonite (PELL, BLOCK):	0.115 0.33, 0.33	0.05
Thermal conductivity wet ($\text{W m}^{-1} \text{K}^{-1}$)	Opalinus Clay (HOST):	2.1	0.1
Thermal conductivity dry ($\text{W m}^{-1} \text{K}^{-1}$)	Opalinus Clay (HOST):	1.4	0.1

4.2 Discussion of selected sensitivity cases

The sensitivity of the simulated pressures at control points P12 through P17 to changes in input parameters is shown as a function of time in Fig. 4-1 and Fig. 4-2, for the sets of reference values given in Tab. 4-1 and Tab. 4-2, respectively.

For times less than 1,000 years, during which the maximum pressures in the surrounding formation occur (see Fig. 3-6), the pressures at P13 through P17 are particularly sensitive to the pore compressibility, pore expansivity, and permeability of the host rock (solid orange line, solid blue line, and dashed orange line, respectively, in Fig. 4-1b-f and Fig. 4-2b-f), but mostly insensitive to other parameters, with a few exceptions as noted next.

For control point P14, which is 50 m above the centre of the waste canister, the pressures are also sensitive to (a) the pore compressibility and (b) the permeability of the nearby formation DOGG (solid brown line and light-blue dashed line in Fig. 4-1c and Fig. 4-2c, respectively). Similarly, for control point P17, which is 50 m below the centre of the waste canister, the pressure is (a) also sensitive to the pore compressibility of nearby ML, AL, and KEUK formations (solid purple, red and green lines, respectively) but (b) less so to the permeability of the corresponding nearby formations (dashed pale-green, grey and pink lines, respectively), as shown in Fig. 4-1f and Fig. 4-2f.

After approximately 1,000 years, in the first reference case that uses high values of pore compressibility for the pedestal and bentonite buffer (see Tab. 4-1) the pressure signal becomes sensitive to the pore compressibility of the pedestal (solid light-blue lines) and bentonite buffer (solid pale-green lines), and sensitivity remains high to the permeability of the host rock (see

Fig. 4-1). In the second reference case which uses lower values of pore compressibility for the pedestal and bentonite buffer (among other differences; see Tab. 4-2) the pressure signal is less sensitive to the pore compressibility of the bentonite pedestal and bentonite buffer but instead has increased sensitivity to the pore expansivity (solid blue line), and sensitivity to the permeability of the host rock remains high (see Fig. 4-2). At later times the pressure sensitivity is complicated by the arrival of pressure wave reflections from the deeper formations and from the model boundaries and is seen to be sensitive to the reference values selected for the analysis.

In general, the pressure waveforms are not sensitive to properties of materials within the tunnel until later times (i.e., until after the maximum pressures occurring in the first peaks of the pressure waveforms at a given control point). Therefore, it is anticipated that, for model calibration, limiting pressure data to that of early times will avoid potential complications arising from the uncertainty in modelling of the inner tunnel properties (e.g., constitutive properties of bentonite clays) (see Fig. 3-6 and corresponding discussion in Section 3.4).

Also note the low sensitivity of the pressure response to the initial porosity – despite the large porosity perturbation values of 0.05. However, it is expected that the function used to calculate changes in porosity has a more substantial influence on the pressure; therefore, parameters that are used in the function that calculates changes in porosity (e.g., pore compressibility and thermal expansivity of the pore space) are selected as parameters to be estimated as part of the THM-TH abstraction.

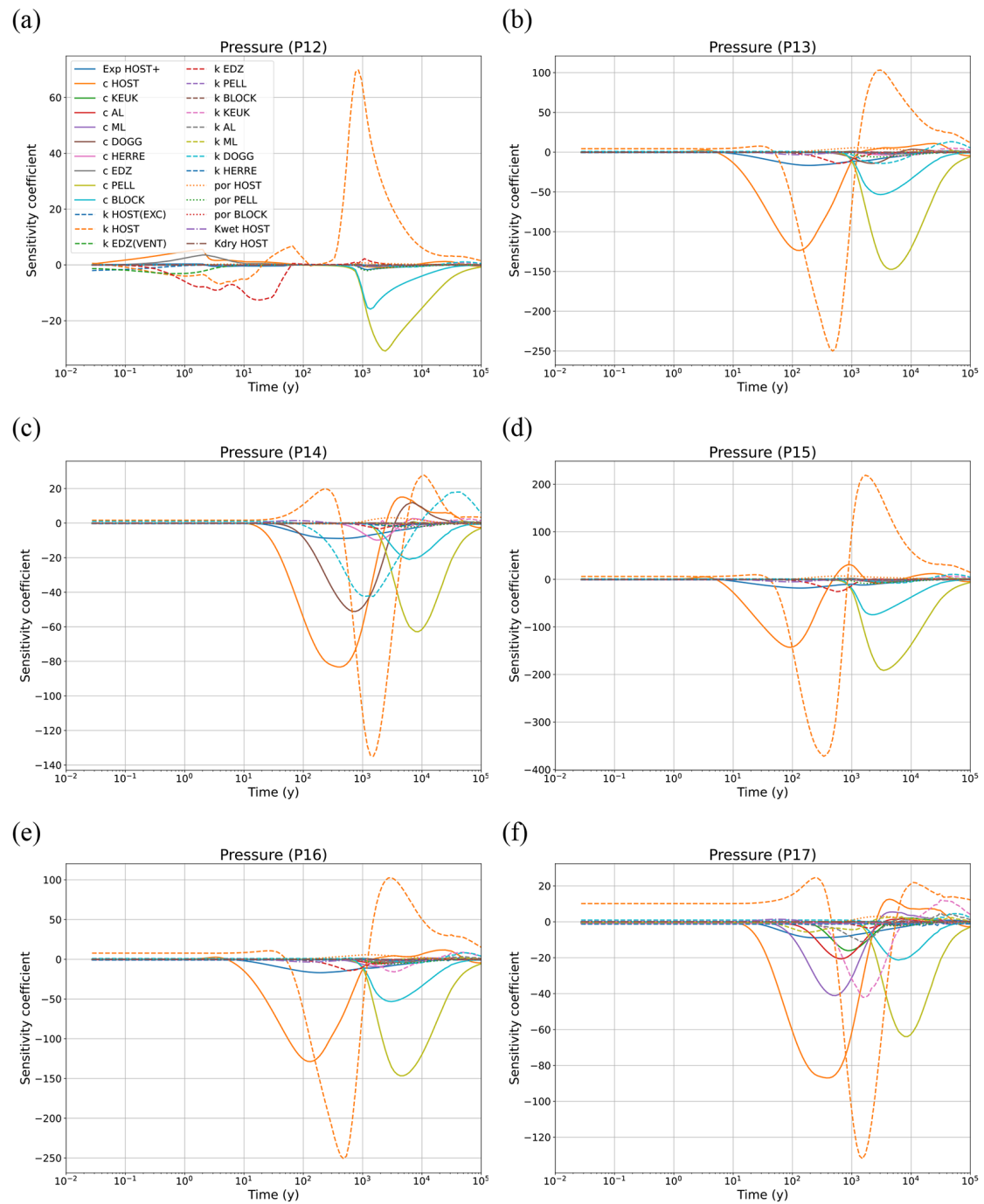


Fig. 4-1: Sensitivity coefficients with reference values based on initial parameters (see Tab. 4-1)

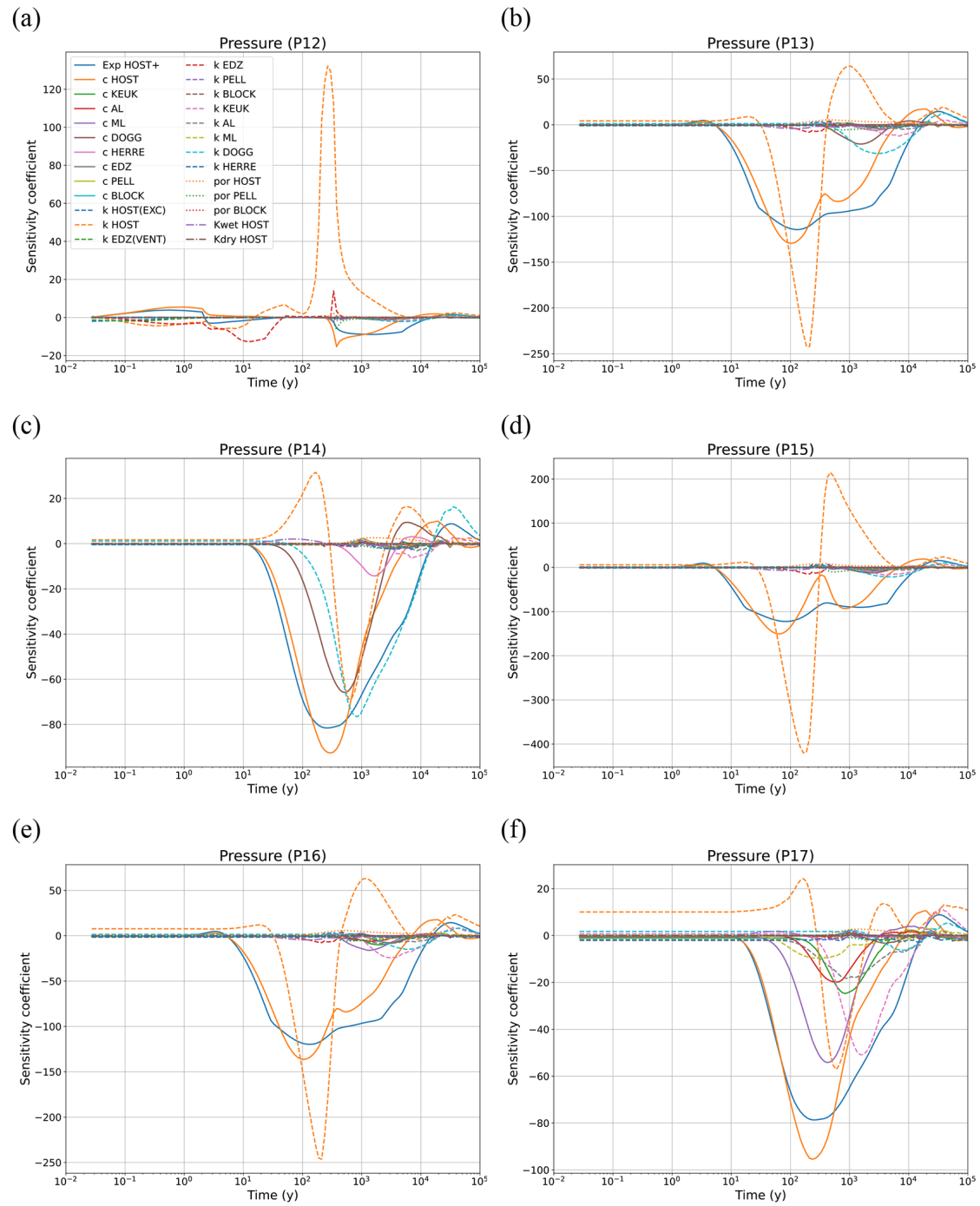


Fig. 4-2: Sensitivity coefficients for pressures with reference values based on calibrated model parameters
(see Tab. 4-2)

5 Estimation of effective parameters

5.1 Approach

A model calibration procedure is performed in which a subset of the iTOUGH2 TH model input parameter values are automatically adjusted (estimated) to obtain an improved match between the simulated observations and the synthetic data generated by the Code_Aster THM model. The resulting calibrated iTOUGH2 model is then able to efficiently reproduce the simulated predictions of interest made by the THM model, such as the maximum pressures in the host rock.

An objective function that quantifies the misfit between simulated model output variables and the synthetic data is defined as follows:

$$S = \sum_{i=1}^m \frac{(z_i^* - z(\mathbf{p})_i)^2}{\sigma_i^2}$$

where z_i^* is synthetic data point i , $z(\mathbf{p})_i$ is the corresponding observation simulated by iTOUGH2 as a function of the input parameter set $\mathbf{p}$, σ_i is the expected standard deviation, reflecting the expected mean residual – which serves to weight the contribution of each data point in the objection function and make different data types comparable – and m is the total number of observations. The expected mean residual reflects what we consider to be an acceptable error for the THM-to-TH abstraction.

The synthetic data considered in this study are the pressures and temperatures at control points P12 through P17 (see Section 5.2 for details). The Levenberg-Marquardt algorithm is used to minimize the objective function and in so doing, identify the parameter set (and related uncertainty estimates) that allows for the best match between the iTOUGH2 model and the synthetic data.

With the goal of keeping the parameterization of the iTOUGH2 model as similar as possible to that of the THM model, the parameters that are adjusted/estimated in this study are limited to two physical properties: pore expansivity and pore compressibility of the materials identified as being influential (see Section 4); it is expected that estimating effective values for these parameters will allow for the THM processes of interest to be sufficiently reproduced by the TH model.

Up to five parameters are estimated, including: log pore compressibility of the host rock, the EDZ, the immediately overlying formation group (referred to as DOGG) and immediately underlying formation (ML); and log pore expansivity of the host rock. The parameter estimates for the considered cases are described in Section 5.3.

No weight is given to prior information of parameters in the objective function, meaning that no preference is given to parameter estimates that are closer to their initially assumed values.

The pressure and temperature data selected as observations for model calibration are shown next (Section 5.2), followed by the inversion results (Section 5.3), and the distributions of pressure, temperature and saturation that are simulated with the final calibrated model (Section 5.4).

5.2 Synthetic data

The pressure and temperature observations that are calculated using the Code_Aster THM model and included as synthetic data for model calibration are shown as symbols in Fig. 5-1 and Fig. 5-2, respectively. The corresponding iTOUGH2 simulation results with the initial and calibrated model are shown as dashed and solid lines, respectively.

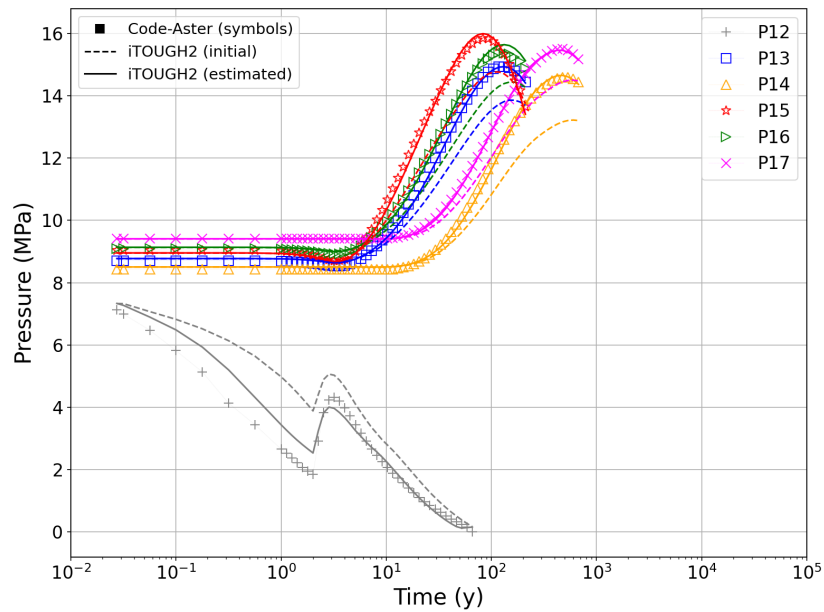


Fig. 5-1: Synthetic pressure data and model fit at P12 through P17, with values simulated by Code_Aster THM model (symbols), and by iTOUGH2 model using initial parameters (dashed lines), and estimated effective parameters (solid lines)

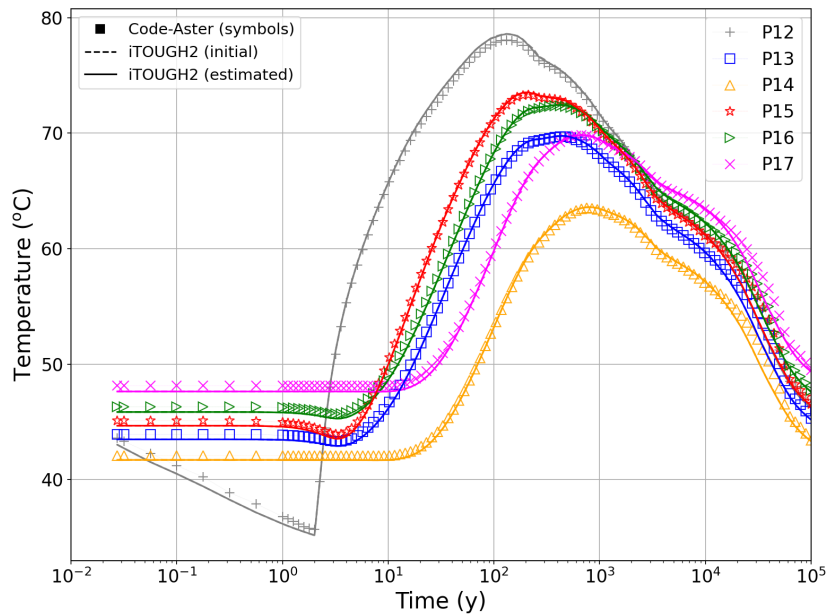


Fig. 5-2: Synthetic temperature data and model fit at P12 through P17, with values simulated by Code_Aster THM model (symbols), and by iTOUGH2 model using initial parameters (dashed lines), and estimated effective parameters (solid lines)

5.2.1 Synthetic time-series data sets

It was concluded in the sensitivity analysis of Section 4 that the pressure response (1) is sensitive to only a few parameters at “early” times (i.e., less than approximately 1,000 years) during which the maximum pressures occur, and (2) is complicated by additional sensitivity to pressure reflections from deeper geological layers and model boundaries, and to bentonite properties, at “later” times (i.e., beyond 1,000 years). Therefore, for model calibration, only pressure observations that occur up to and slightly after the maximum pressures (i.e., the “first peaks” in pressure) at their respective control points P13 through P17 are included as synthetic data; a more limited time range is used for P12 (see Fig. 5-1). For temperature observations, all times are included as synthetic data for model calibration (see Fig. 5-2), although it is noted that they had limited sensitivity to the effective parameters that were ultimately estimated by inverse modelling.

Details of the synthetic pressure data sets, including number of times, time range, and assumed measurement errors are given in Tab. 5-1. The same standard deviation value of 0.05 MPa is assumed for data sets at P13 through P17, while that value is increased by a factor of 10 ($\sigma_{p, P12} = 0.5$ MPa) for P12, which serves to give less weight to P12 and keep it from having an undue effect on model calibration results (i.e., it is preferred not to excessively improve the fit at P12, which is in the immediate vicinity of the tunnel), at the expense of the fit to the observations at more distant positions, for which accurate predictions are more important. The sensitivity of inversion results to the number of pressure data at P12 and the weight assigned to them is considered in Section 5.3.2 and 5.3.3.

Tab. 5-1: Description of synthetic time-series pressure data and residuals for base-case model calibration described in Section 5.3.1

(see Tab. 5-4 and Fig. 5-1)

Observation	Number of times	$t_{\min}$ [days]	$t_{\max}$ [yr]	Assumed σ_P [Mpa]	Residuals μ_P [Mpa]	Residuals σ_P [Mpa]
Pressure at P12	44	10	65.8	0.5	-0.18	0.39
Pressure at P13	54	10	210.5	0.05	0.017	0.11
Pressure at P14	64	10	673.4	0.05	-0.006	0.10
Pressure at P15	54	10	210.5	0.05	0.073	0.12
Pressure at P16	54	10	210.5	0.05	-0.052	0.11
Pressure at P17	64	10	673.4	0.05	0.013	0.03

A similar breakdown of the synthetic temperature data sets is given in Tab. 5-2. Note that all temperature data cover a time span of 100,000 years and assume the same value for measurement error ($\sigma = 1^\circ\text{C}$).

Tab. 5-2: Description of synthetic time-series temperature data and residuals for base-case model calibration described in Section 5.3.1

(see Tab. 5-4 and Fig. 5-2)

Observation	Number of times	$t_{\min}$ [days]	$t_{\max}$ [yr]	Assumed σ_P [Mpa]	Residuals μ_P [Mpa]	Residuals σ_P [Mpa]
Temperature at P12	107	10	1.0e5	1.0	0.048	0.63
Temperature at P13	107	10	1.0e5	1.0	0.28	0.48
Temperature at P14	107	10	1.0e5	1.0	0.27	0.44
Temperature at P15	107	10	1.0e5	1.0	0.24	0.50
Temperature at P16	107	10	1.0e5	1.0	0.27	0.46
Temperature at P17	107	10	1.0e5	1.0	0.34	0.40

5.2.2 Synthetic maximum (or peak) pressure data set

It is also of interest to know whether a reduced pressure data set that includes only maximum pressures (or peak pressures) can be used successfully in the model calibration procedure instead of the time-series pressure data. Maximum pressures (i.e., the “first peaks” in pressure) occurring at control points P13 through P17, in addition to the maximum pressure occurring at control point P12 between 2 and 70 years, are recorded and included in a synthetic maximum-pressure data set (see Tab. 5-3).

For the maximum pressures at P13 through P17, a standard deviation of 0.0003 MPa is assumed; this value is decreased relative to that assumed for the time-series pressure data (0.05 MPa) to provide a similar weight to the pressure data (of which there are six or fewer maximum pressure

calibration points) relative to that of the temperature data (of which there are 642 calibration points) in the objective function. The maximum pressure at P12 is either given an increased standard deviation, or it is removed from the dataset entirely, to highlight its effect of the performance of the model calibration in the inversion results described in Section 5.3.3.

Tab. 5-3: Description of synthetic maximum-pressure data and residuals for the model calibration described in Section 5.3.3 that assumes $\sigma_{P, P12} = 3 \times \sigma_{P, P13-17}$ (see Tab. 5-9 and Fig. 5-4)

Observation	Number of points	$t_{\min}$ [days]	$t_{\max}$ [yr]	Assumed σ_P [Mpa]	Residuals μ_P [Mpa]
Max. Pressure at P12	1	735	70	0.0009	-0.041
Max. Pressure at P13	1	10	100,000	0.0003	0.1188
Max. Pressure at P14	1	10	100,000	0.0003	0.0028
Max. Pressure at P15	1	10	100,000	0.0003	-0.0097
Max. Pressure at P16	1	10	100,000	0.0003	-0.095
Max. Pressure at P17	1	10	100,000	0.0003	0.0056

5.3 Inversion results

The base-case inversion that uses synthetic time series pressure and temperature data is described in Section 5.3.1. This inversion results in the calibrated model that is subsequently used as a basis for prediction uncertainty analysis.

Sensitivity of the inversion results to the assumed level of uncertainty (or weight) assigned to the pressures in the EDZ at control point P12 is examined in Section 5.3.2.

In Section 5.3.3, the inversion performance of a potential scenario that uses a simplified, reduced form of pressure data, namely the maximum (or peak) pressures at each control point, instead of the time series pressures, is evaluated.

5.3.1 Inversion with synthetic time series data

For the base-case, an iTOUGH2 inversion was conducted with 16 successful iterations (parameter updates) that reduced the objective function from its initial value of 5.65e4 (corresponding to the initial parameter guesses), down to a value of 1.5e3, or 2.7% of the initial value (for the final estimated parameter set). The estimated error variance (a measure of the mean residual in comparison to the assumed standard deviations shown in Tab. 5-1 and Tab. 5-2) is 1.55, which, being slightly greater than 1.0, indicates that the match is not quite as good as expected but can be considered acceptable.

In Fig. 5-1 and Fig. 5-2, the pressure and temperature observations, respectively, are shown for the initial iTOUGH2 model (dashed lines), the final calibrated model (solid lines), together with the respective synthetic data (symbols). The calibrated model generally gives a very good fit to the synthetic data.

The means and standard deviations of the residuals for each pressure and temperature data set are listed in Tab. 5-1 and Tab. 5-2, respectively, and are mostly in line with expectations. The average of the residuals (indicative of a potential systematic bias) for the pressure data sets is -0.017 MPa, with P12 showing the largest residual. The average of the standard deviations of the pressure residuals is (a) 0.39 MPa for P12, which is less than the assumed value of 0.5 MPa, and (b) 0.09 for P13 – P17, which slightly exceeds the assumed value of 0.05 MPa.

The average of the standard deviations of the temperature residuals for P12 through P17 is 0.5 °C, which is less than the assumed value of 1.0 °C. While accuracy of temperature data is slightly underpredicted, there is a slight bias in the residuals (with temperatures overpredicted on average by about 0.24 °C); this bias may be related to slight differences in the implementation of boundary conditions between the Code_Aster and iTOUGH2 models.

The estimated parameter values and standard deviations can be found in Tab. 5-4. Notably, the uncertainty estimates are low, ranging between 0.006 and 0.06, reflecting the overall excellent fit to the synthetic data. For the host rock, the estimated value of log pore expansivity is increased substantially compared to its initial value (from -4.77 to -3.84), while the log pore compressibility is decreased from -8.77 to -9.14. The estimated pore compressibility values for most of the remaining materials (ML, DOGG) are not dramatically different from their original values; the value for the EDZ is reduced substantially from -8.35 to -9.37.

There is also a measure of parameter estimation independence reported in Tab. 5-4, specifically the ratio of the conditional standard deviation (estimation uncertainty assuming all other parameters are perfectly known) to the marginal standard deviation (estimation uncertainty that accounts for correlation between parameters). The C/M values for estimated log pore compressibility values of the EDZ, ML and DOGG materials are close to 1 (between 0.8 and 0.94), indicating that their estimation is relatively independent of the other parameters. Conversely, the C/M values for the log pore compressibility and log pore expansivity of the host rock are lower (0.18), as they are (negatively) correlated with each other (see Tab. 5-5).

Tab. 5-4: Results of base-case inversion with synthetic time series data for P12 through P17, to be used as the basis for parameter uncertainty analysis in Section 6

Assumes $\sigma_{p, P12} = 10 \times \sigma_{p, P13-17}$ (as defined in Tab. 5-1). Estimated error variance $\sigma_o^2 = 1.55$

Parameter	Material	Initial	Estimate	Std. Dev.	C/M	Sens. OBJ
$\log_{10}$ (pore expansivity (1/°C))	HOST	-4.770	-3.842	6.7e-3	0.18	2,128
$\log_{10}$ (pore compressibility (1/Pa))	HOST	-8.766	-9.141	5.7e-3	0.18	3,143
	EDZ	-8.352	-9.368	0.059	0.80	27
	ML	-8.796	-8.862	7.9e-3	0.87	79
	DOGG	-8.853	-9.051	5.7e-3	0.94	139
	BLOCK	-10.0	<i>fixed</i>	N/A	N/A	N/A
	PELL	-10.0	<i>fixed</i>	N/A	N/A	N/A

The covariance matrix and correlation coefficients of the estimated parameter set are shown in Tab. 5-5, with the diagonal elements representing the variances, the lower triangular matrix the covariances, and the upper elements the correlation coefficients.

Note the high negative correlation (-0.97) between the pore compressibility and pore expansivity of the host. The next highest correlation occurs between the pore compressibility of the EDZ and that of the ML material, but the sensitivity of the objective function to those two parameters is low (see final column in Tab. 5-4, which shows the sensitivity of the objective function with respect to each parameter). Correlations among the remaining parameters is generally low, with absolute values between 0.01 and 0.14.

Tab. 5-5: Covariance(L+D)/Correlation(U) matrix for inversion of synthetic time series data

Parameter with “exp [material]” refer to $\log_{10}$ (pore expansivity (1/°C)), and those with “c [material]” refer to $\log_{10}$ (pore compressibility (1/Pa))

Parameters	exp HOST	c ML	c DOGG	c HOST	c EDZ
exp HOST	4.53e-5	0.108	0.085	-0.976	0.011
c ML	5.74e-6	6.22e-5	0.105	-0.143	-0.342
c DOGG	3.24e-6	4.69e-6	3.20e-5	-0.144	-0.044
c HOST	-3.71e-5	-6.37e-6	-4.59e-6	3.19e-5	-0.097
c EDZ	4.27e-6	-1.58e-4	-1.47e-5	-3.22e-5	3.42e-3

5.3.2 Sensitivity of inversion to uncertainty in time series pressures at P12

During early model calibration efforts, results were found to be sensitive to the uncertainty assigned to synthetic pressure data at control point P12. These pressure data are in the EDZ near the tunnel and have a distinctly different character than those at control points P13 through P17 (e.g., see Fig. 3-6), which are at least 20 m away. Note that the uncertainty assigned to individual data points determines the amount of weight that is given to them in model calibration (i.e., the weight is given by the inverse of the assumed standard deviation) and thus affects their influence on the inversion results. Inversion performance was also found to deteriorate when these synthetic data at P12 were excluded entirely from the model calibration or given no weight.

As discussed previously, the standard deviation for pressures at P12 ($\sigma_{P, P12}$) in the base-case inversion was assumed to be 10 times greater than that for the pressures at P13-P17 ($\sigma_{P, P13-17}$). Additional inversions were performed to examine the sensitivity of results to this input specification. Specifically, inversions were performed with $\sigma_{P, P12}$ set to values of 1, 3, 10, or 20 times greater than $\sigma_{P, P13-17}$. All inversions use the same initial parameter guesses.

Fig. 5-3 shows the pressures simulated with the resulting models, with the largest variations between cases most evident in the pressures at P12 (solid and dashed grey lines). While the estimated values and standard deviations are similar to those of the base-case inversion for most parameters (e.g., estimates of the log pore expansivity and log pore compressibility are shown in Tab. 5-6 and Tab. 5-7, respectively), the estimates for the log pore compressibility of the EDZ material vary substantially (between -9.3 and -11.7), as do the standard deviations (between 0.039 and 0.12) (see Tab. 5-8). The error variance is highest (4.1) for the case that assumes the highest level of accuracy for P12 pressure data ($\sigma_{P, P12} = \sigma_{P, P13-17} = 0.05$ MPa), which is consistent with the fact that the standard deviation of the pressure residuals at P12 remains relatively large (0.35 MPa) for this case. The cases with the lowest error variance, around 1.5, assume $\sigma_{P, P12} = 10 \times \sigma_{P, P13-17} = 0.5$ MPa (the base-case inversion) and $\sigma_{P, P12} = 20 \times \sigma_{P, P13-17} = 1.0$ MPa, resulting in pressure

residuals of 0.18 MPa and 0.46 MPa, respectively. Overall, these sensitivity results show consistency between cases and confirm the suitability of the input specification that was selected for the base-case inversion ($\sigma_{P, P12} = 10 \times \sigma_P$).

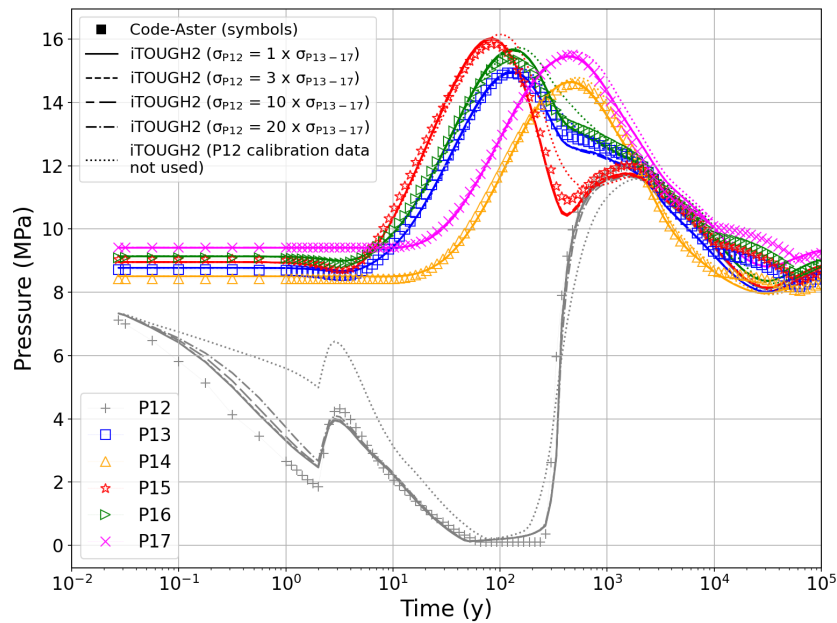


Fig. 5-3: Pressures simulated with iTOUGH2 models that were calibrated using time series pressures compared with values simulated by Code_Aster model (symbols)

Calibrations assume that (a) uncertainty in the pressures at P12 (sp, P12) are a multiple of the assumed uncertainty for P13 through P17 (sp, P13-17) (indicated by the lines shown in the legend), or (b) calibration data points at P12 are excluded from calibration (dotted lines)

Tab. 5-6: Sensitivity of HOST log pore expansivity estimate to P12 time series data

Sensitivity case	σ_o^2	$\log_{10}$ (pore expansivity (1/°C)) of HOST		
		Estimate	Std. Dev.	C/M
$\sigma_{P, P12} = \sigma_{P, P13-17}$	4.05	-3.829	7.4e-3	0.25
$\sigma_{P, P12} = 3 \times \sigma_{P, P13-17}$	1.80	-3.841	6.6e-3	0.20
$\sigma_{P, P12} = 10 \times \sigma_{P, P13-17}$	1.55	-3.842	6.7e-3	0.18
$\sigma_{P, P12} = 20 \times \sigma_{P, P13-17}$	1.53	-3.847	7.1e-3	0.18
No data at P12 used	4.90	-4.779	0.079	0.28

Tab. 5-7: Sensitivity of HOST log pore compressibility estimate to P12 time series data

Sensitivity case	σ_o^2	$\log_{10}$ (pore compressibility (1/Pa)) of HOST		
		Estimate	Std. Dev.	C/M
$\sigma_{P, P12} = \sigma_{P, P13-17}$	4.05	-9.158	6.7e-3	0.24
$\sigma_{P, P12} = 3 \times \sigma_{P, P13-17}$	1.80	-9.143	5.6e-3	0.19
$\sigma_{P, P12} = 10 \times \sigma_{P, P13-17}$	1.55	-9.141	5.7e-3	0.18
$\sigma_{P, P12} = 20 \times \sigma_{P, P13-17}$	1.53	-9.138	5.8e-2	0.17
No data at P12 used	4.90	-8.91	5.0e-3	0.29

Tab. 5-8: Sensitivity of EDZ log pore compressibility estimate to P12 time series data

Sensitivity case	σ_o^2	$\log_{10}$ (pore compressibility (1/Pa)) of EDZ		
		Estimate	Std. Dev.	C/M
$\sigma_{P, P12} = \sigma_{P, P13-17}$	4.05	-11.68	0.12	0.99
$\sigma_{P, P12} = 3 \times \sigma_{P, P13-17}$	1.80	-11.54	5.6e-2	0.80
$\sigma_{P, P12} = 10 \times \sigma_{P, P13-17}$	1.55	-9.87	5.9e-2	0.80
$\sigma_{P, P12} = 20 \times \sigma_{P, P13-17}$	1.53	-9.26	3.9e-2	0.74
No data at P12 used	4.90	-10.11	0.23	0.99

Another conceivable inversion strategy is to exclude the synthetic data at P12 from model calibration if its uncertainty were deemed unacceptably high (or due to concern about unresolved systematic errors in nearfield pressures between the iTOUGH2 TH and Code_Aster TH model, as discussed in Section 3.2). However, in this example, it is shown that model calibration performed without the P12 data results in a significantly deteriorated data fit for pressures at P12 through P17 (dotted lines in Fig. 5-3) and poor parameter estimates (see Tab. 5-6, Tab. 5-7 and Tab. 5-8). It should be noted that, in this case, the optimization algorithm encountered a local minimum in the objective function and failed to find the global minimum, due to increased non-uniqueness in the inverse problem resulting from removal of the P12 data set from the calibration procedure.

5.3.3 Inversions with maximum pressures (and times series temperatures)

An alternative approach for model calibration is also considered in which a simplified, reduced form of the pressure data is used, namely the maximum “peak” pressure occurring at each control point, instead of the synthetic time series data.

Fig. 5-4 shows the simulated pressures for three inversion cases with different assumptions made about the maximum-pressure data at P12, including ones that assume the uncertainty for P12 pressure data is three times and 10 times that of the maximum pressure data for P13 through P17 (solid and dashed lines, respectively), and one that excludes the maximum pressure data at P12 from model calibration altogether (dotted lines). It should be noted that each inversion uses the same initial parameter guesses. Further details are given in Tab. 5-9, Tab. 5-10, and Tab. 5-11 for the respective cases.

The results are found to be especially sensitive to the weight assigned to the maximum pressure at P12 (Fig. 5-4). Note that the predictions of the time-series pressures are (1) unsurprisingly not as good as for the cases in which the time-series pressures are used in calibration (see Fig. 5-3), and (2) best overall, including at P13 through P17, for the case in which the highest amount of weight (lowest uncertainty) is assigned to the maximum-pressure calibration point at P12.

Even for the best of the maximum-pressure inversions, a higher degree of parameter correlation is observed (Tab. 5-12) than for the base-case inversion that uses time-series pressures (Tab. 5-5).

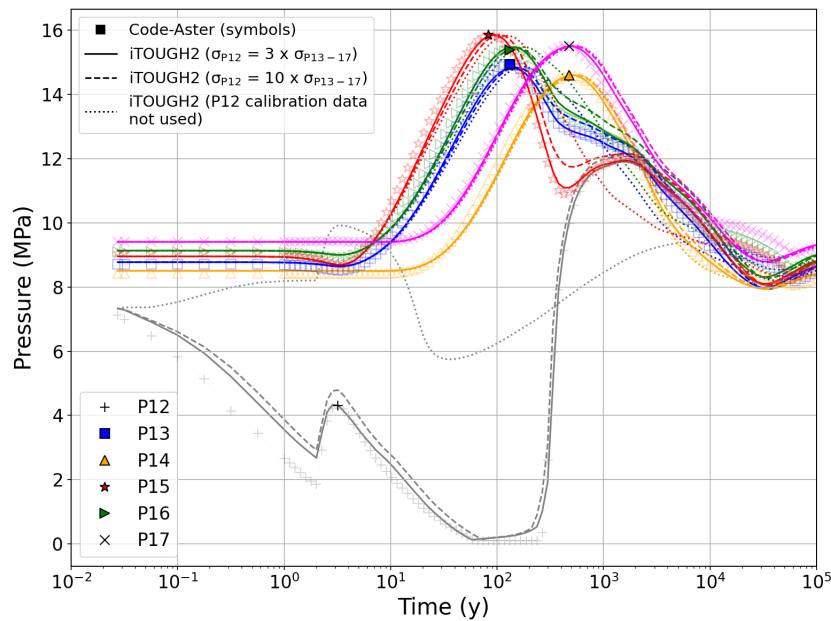


Fig. 5-4: Pressures simulated with iTOUGH2 models that were calibrated using a limited number of maximum “peak” pressures (solid/dark symbols) compared with pressures simulated by Code_Aster model (light symbols)

Calibrations assume that (a) uncertainty in the maximum pressure at P12 ($\sigma_{p, P12}$) is (a) 3 or (b) 10 times higher than for P13 through P17 ($\sigma_{p, P13-17}$) (solid lines), or (c) the calibration data point at P12 is excluded from calibration (dotted lines)

Tab. 5-9: Results of inversion with maximum pressures and temperature time series data for P12 through P17, assuming $\sigma_{p, P12} = 3 \times \sigma_{p, P13-17}$

Estimated error variance $\sigma_o^2 = 2.05$

Parameter	Material	Initial	Estimate	Std. Dev.	C/M	Sens. OBJ
$\log_{10}$ (pore expansivity (1/°C))	HOST	-4.770	-4.056	0.009	0.10	1,767
$\log_{10}$ (pore compressibility (1/Pa))	HOST	-8.766	-8.998	0.004	0.10	12,213
	EDZ	-8.352	-10.69	0.06	0.99	3
	ML	-8.796	-8.945	0.004	0.83	188
	DOGG	-8.853	-9.08	0.002	0.91	457
	BLOCK	-10.0	<i>Fixed</i>	N/A	N/A	N/A
	PELL	-10.0	<i>Fixed</i>	N/A	N/A	N/A

Tab. 5-10: Results of inversion with maximum pressures and temperature time series data for P12 through P17, assuming $\sigma_{p, P12} = 10 \times \sigma_{p, P13-17}$

Estimated error variance $\sigma_o^2 = 1.98$

Parameter	Material	Initial	Estimate	Std. Dev.	C/M	Sens. OBJ
$\log_{10}$ (pore expansivity (1/°C))	HOST	-4.770	-5.45	0.067	0.43	93
$\log_{10}$ (pore compressibility (1/Pa))	HOST	-8.766	-8.859	6.0e-4	0.59	15,119
	EDZ	-8.352	-9.33	0.058	0.48	108
	ML	-8.796	-9.014	0.005	0.85	75
	DOGG	-8.853	-9.117	0.003	0.91	194
	BLOCK	-10.0	<i>Fixed</i>	N/A	N/A	N/A
	PELL	-10.0	<i>Fixed</i>	N/A	N/A	N/A

Tab. 5-11: Results of inversion with maximum pressures and temperature time series data for P13 through P17 (synthetic data at P12 not used)

Estimated error variance $\sigma_o^2 = 1.65$

Parameter	Material	Initial	Estimate	Std. Dev.	C/M	Sens. OBJ
$\log_{10}$ (pore expansivity (1/°C))	HOST	-4.770	-6.074	0.087	0.12	26
$\log_{10}$ (pore compressibility (1/Pa))	HOST	-8.766	-8.828	0.052	0.06	14,827
	EDZ	-8.352	-6.51	0.12	0.15	61
	ML	-8.796	-9.124	0.026	0.19	140
	DOGG	-8.853	-9.172	0.011	0.21	314
	BLOCK	-10.0	<i>fixed</i>	N/A	N/A	N/A
	PELL	-10.0	<i>fixed</i>	N/A	N/A	N/A

Tab. 5-12: Covariance(L+D)/Correlation(U) matrix for inversion of maximum pressures

Inversion assumes $\sigma_{p, P12} = 3 \times \sigma_{p, P13-17}$. Parameters with “exp [material]” refer to $\log_{10}$ (pore expansivity (1/°C)), and those with “c [material]” refer to $\log_{10}$ (pore compressibility (1/Pa))

Parameters	exp HOST	c ML	c DOGG	c HOST	c EDZ
exp HOST	2.93e-5	0.492	0.329	-0.994	-0.110
c ML	6.20e-6	5.42e-6	0.257	-0.519	-0.056
c DOGG	2.38e-6	7.98e-7	1.78e-6	-0.356	0.029
c HOST	-1.18e-5	-2.67e-6	-1.05e-6	4.88e-6	0.112
c EDZ	-1.88e-5	-4.12e-6	1.21e-6	7.86e-6	1.01e-3

5.4 Objective function

As described in Section 5.1, the objective function is a measure of the misfit between the pressure and temperature observations simulated by the iTOUGH2 model and the corresponding synthetic data generated by the Code_Aster THM model; it is a multi-dimensional function of the input parameters.

The objective function for the calibrated model of this study (see Fig. 5-1 and Fig. 5-2; Tab. 5-4, and discussion in Section 5.3.1) is visualized through the two-dimensional parameter sub-space as a function of the two most influential parameters in the model calibration, the log pore compressibility and log pore expansivity of the host rock, in Fig. 5-5a. The remaining parameters have low correlation with the pore compressibility and pore expansivity parameters and are fixed to the values that were estimated in model calibration.

In addition, 1-D slices of each parameter passing through the minimum of the objective function are shown in Fig. 5-5b; specifically, the log pore compressibility versus the objective function is plotted for a log pore expansivity value of $-3.84 \log_{10}[1/°C]$, while the log pore expansivity versus the objective function is plotted for a log pore compressibility value of $-9.14 \log_{10}[1/Pa]$.

Similar, expanded views of the objective function are shown in Fig. 5-6, including the approximate estimation uncertainty (confidence region), shown with a white line in Fig. 5-6a. The confidence region is a level of the objective function that is calculated based on the estimated error variance, the number of parameters, the degree of freedom in the inverse problem, and a quantile of the F-distribution (see Finsterle 2007).

Inspection of the objective function generally shows that despite non-uniqueness in the inverse solution due to correlation between the pore compressibility and pore expansivity, the synthetic data are sufficiently sensitive to obtain a unique solution with low estimation uncertainty.

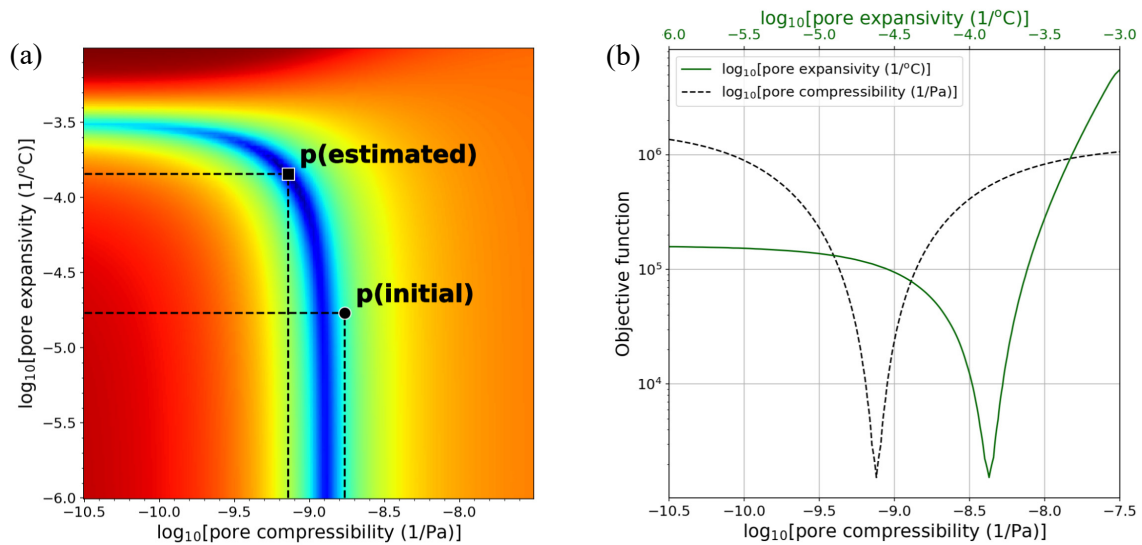


Fig. 5-5: Visualization of the objective function

calculated (a) in 2-D parameter sub-space for log pore compressibility versus log pore expansivity in the host rock, and (b) for 1-D slices of each parameter passing through the minimum of the objective function. The initial parameter set and final estimated parameter set are indicated by a black circle and square, respectively, in (a).

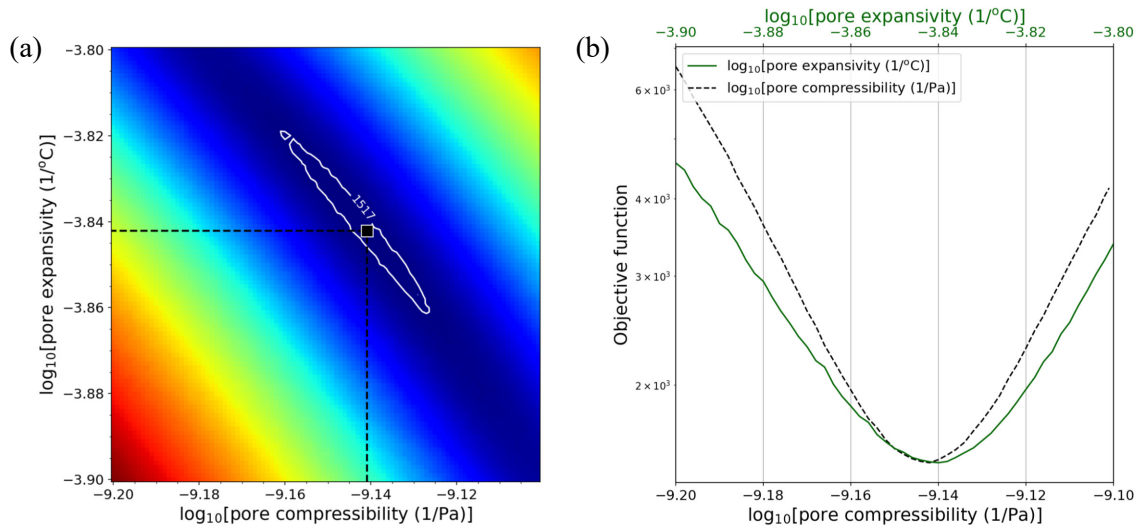


Fig. 5-6: Visualization of the objective function (expanded view)

calculated (a) in 2-D parameter sub-space for log pore compressibility versus log pore expansivity in the host rock, and (b) for 1-D slices of each parameter passing through the minimum of the objective function. In (a), the final estimated parameter set is indicated by a black square and the confidence region is shown with a white contour line.

It is also worth noting that inversion results were sensitive to the numerical accuracy of the TH simulation, specifically the TOUGH2 parameter RE1, which specifies the convergence criterion for relative error (see Pruess 2012). Depictions of the calculated objective function show that fluctuations due to numerical inaccuracy are substantial for $RE1 = 10^{-4}$ (Fig. 5-7a), decreased but still apparent for $RE1 = 10^{-5}$ (Fig. 5-7b), and low for $RE1 = 10^{-6}$ (Fig. 5-7c). Therefore, an RE1 value of 10^{-6} was used for final model calibrations.

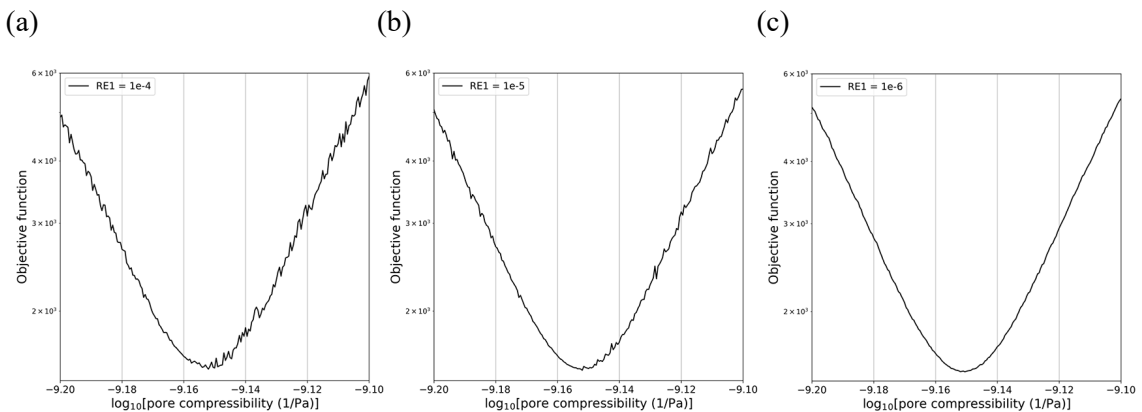


Fig. 5-7: Sensitivity of calculated objective function to numerical accuracy of simulation
TOUGH2 relative error convergence criteria parameter RE1: (a) 10^{-4} , (b) 10^{-5} , (c) 10^{-6}

5.5 Simulated distributions

The evolution of the saturation, temperature and pressure distributions is simulated with the calibrated iTOUGH2 model. Close-up views of the distribution of these simulated system states within the tunnel are shown in Fig. 5-8, Fig. 5-9, and Fig. 5-10, respectively. In addition, an expanded view of the pressure is shown in Fig. 5-11, for the entire width of the model.

The response is consistent with what is seen in the THM simulation (and described in Appendix A). Increased temperatures due to heating in the HLW canister lead to increases in pressure in the host rock, while the pressure remains relatively lower in the tunnel (and the EDZ) due to lingering effects from the period in which the tunnel was open to the atmosphere and the bentonite was unsaturated. Wetting of the bentonite materials proceeds slowly, with a saturation front moving upward in the bentonite pedestal and inward from the concrete liner through the bentonite buffer. The pressures inside the tunnel and in the liner eventually increase as they become saturated with water by approximately 300 years.

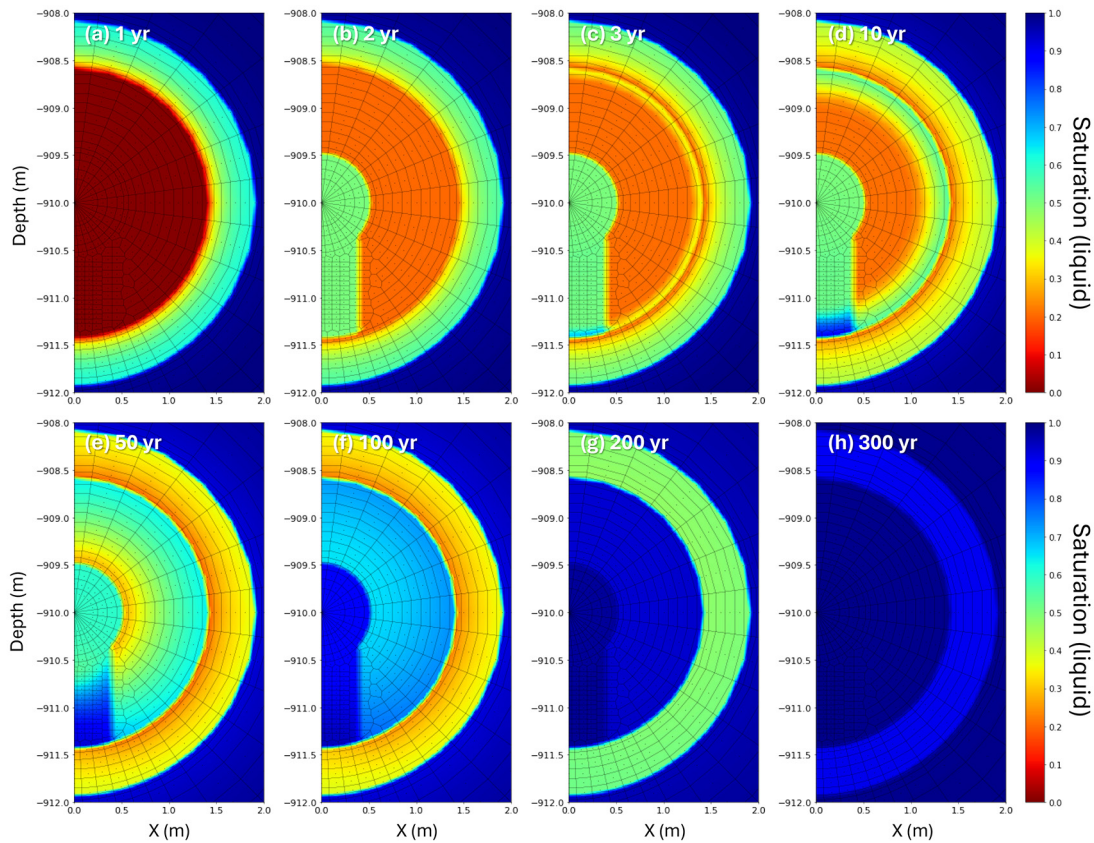


Fig. 5-8: Simulated liquid saturation distributions at various times

(a) 1 yr, (b) 2 yr, (c) 3 yr, (d) 4 yr, (e) 50 yr, (f) 100 yr, (g) 200 yr, and (h) 300 yr. Near-tunnel view ($X < 2$ m).

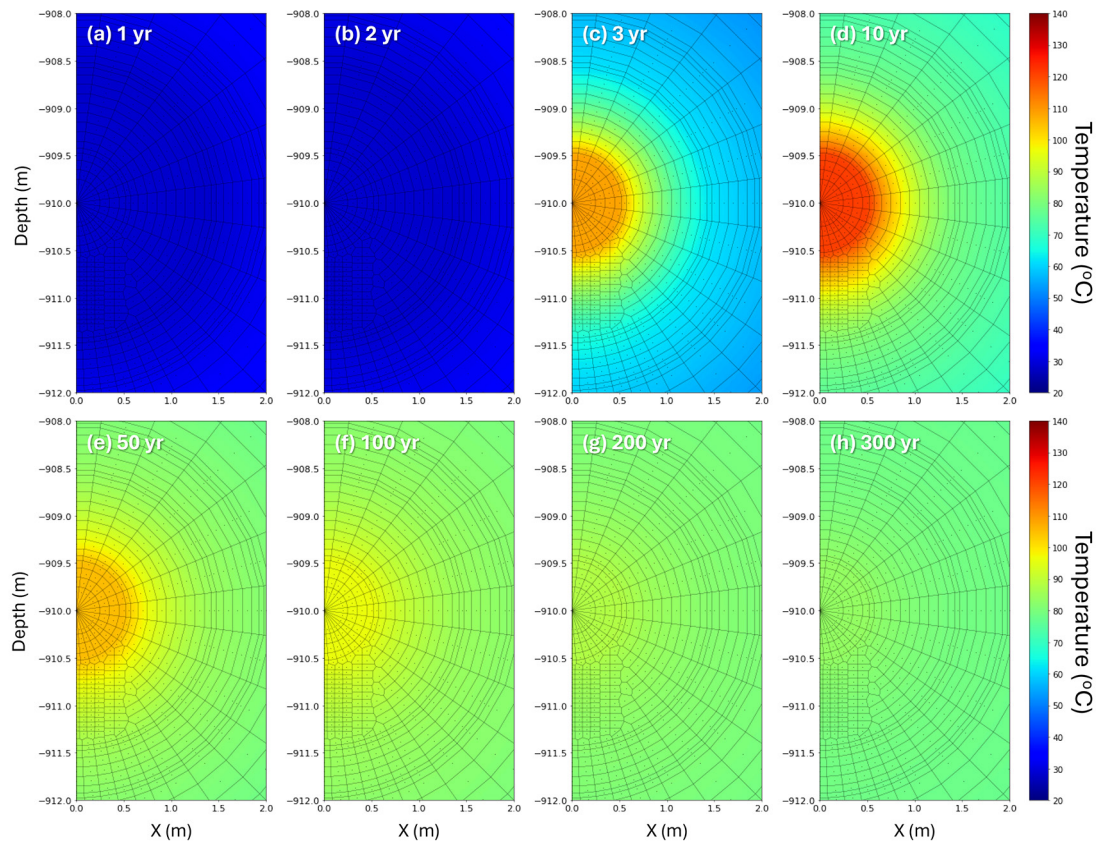


Fig. 5-9: Simulated temperature distributions at various times

(a) 1 yr, (b) 2 yr, (c) 3 yr, (d) 4 yr, (e) 50 yr, (f) 100 yr, (g) 200 yr, and (h) 300 yr. Near-tunnel view ($X < 2$ m).

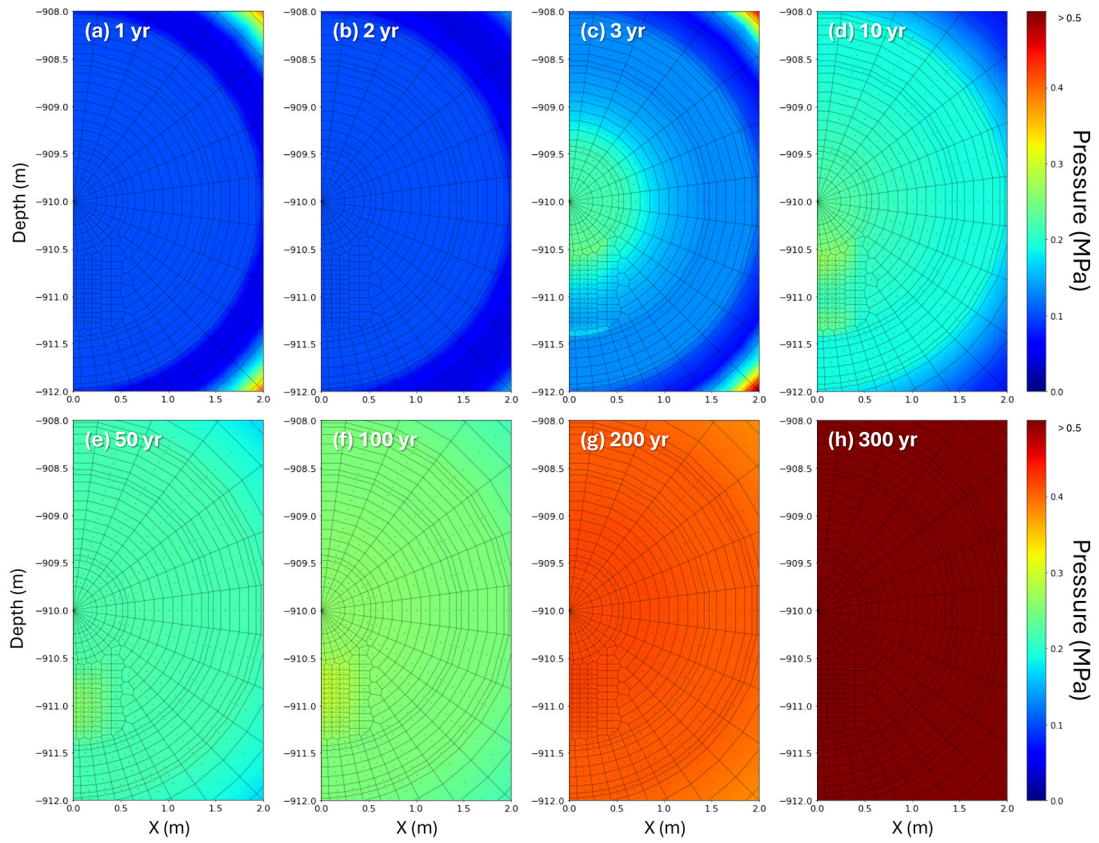


Fig. 5-10: Simulated pressure distributions at various times

(a) 1 yr, (b) 2 yr, (c) 3 yr, (d) 4 yr, (e) 50 yr, (f) 100 yr, (g) 200 yr, and (h) 300 yr. Near-tunnel view ($X < 2$ m). Note that different times are shown than in Fig. 5-11, which highlights pressure evolution further from the tunnel at longer time scales.

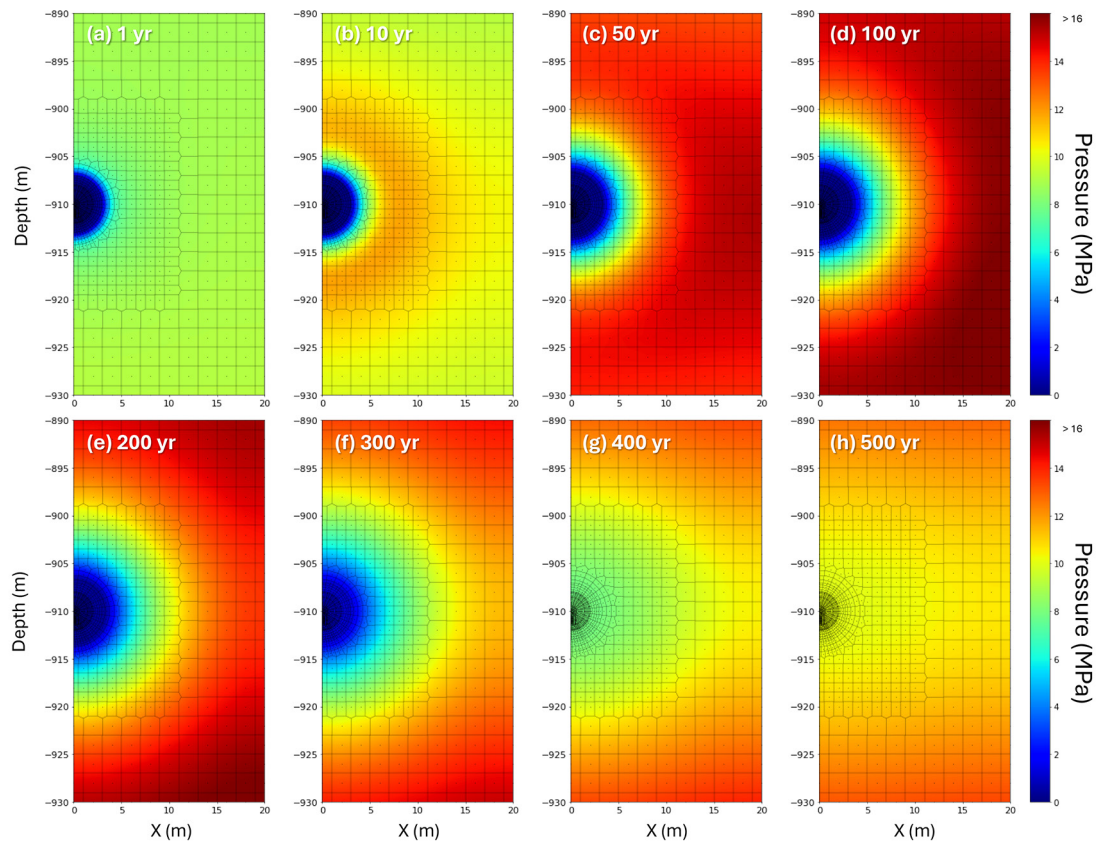


Fig. 5-11: Simulated pressure distributions, showing a view of the full model width (but limited depth range), at various times

(a) 1 yr, (b) 10 yr, (c) 50 yr, (d) 100 yr, (e) 200 yr, (f) 300 yr, (g) 400 yr, and (h) 500 yr. Note that different times are shown than in Fig. 5-10, which highlighted pressure evolution within the tunnel at shorter time scales.

6 Prediction uncertainty analysis

6.1 Approach

The impact of potential sources of uncertainty in the iTOUGH2 model on predictions of interest – namely the pressures at control points P12 through P17 – is evaluated through Monte Carlo simulations with Latin Hypercube Sampling (Zhang & Pinder 2003). The procedure is performed with iTOUGH2 as follows: (1) parameters are selected and their uncertainty is defined through probability density functions (pdfs); (2) parameter values are sampled from the respective pdfs to create parameter vectors; (3) an iTOUGH2 simulation is performed using the given parameter vector as input, and the resulting observations are stored; (4) steps (2) and (3) are repeated for a number of realizations; and (5) the ensemble of simulation results is analysed.

The base-case calibrated iTOUGH2 model described earlier (in Section 5.3.1), using effective parameters determined through model calibration, is used as the basis for prediction uncertainty analyses. While this model was calibrated using pressures at a limited number of times (see Fig. 5-1), the pressure fits at later times are generally good as well (except for slight differences arising after 10^4 years due to effects from the lower boundary), as shown in Fig. 6-1.

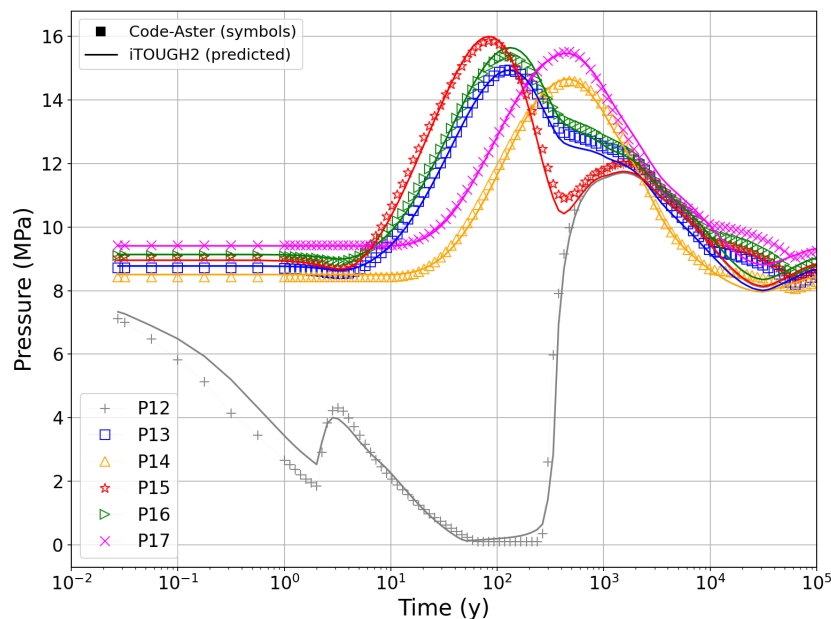


Fig. 6-1: Comparison of pressure profiles from the original Code_Aster THM simulation and predictions made with the final calibrated iTOUGH2 model

Several uncertainty propagation analyses are presented. The first, which may also be considered a sensitivity analysis, is intended to illustrate the way in which different parameter sets influence model predictions. In the second, the impact of the actual estimation uncertainty in the model abstraction process on prediction uncertainty is evaluated, and additional variations are considered with more conservative assumptions about uncertainty. Finally, a third analysis demonstrates the impact of overall model uncertainty that is expected to be relevant – not in the model abstraction step, but in general applications of the model, where additional sources of

uncertainty exist (e.g., uncertainty in permeability of geological formations) that are expected to influence prediction uncertainty more than the uncertainty resulting from the model abstraction step alone.

6.2 Analysis 1 – Illustration of parameter influence on prediction uncertainty (not based on calibrated model)

While this first case is not technically based on the calibrated version of iTOUGH2 model, it is included nonetheless to illustrate the way in which different sets of effective TH parameters influence model predictions as they are varied in the THM to TH model abstraction process. This is accomplished by sampling from uniform pdfs that are not centred around the best parameter estimates from model calibration; rather, the extreme values of the uniform pdfs are defined by (a) the original values specified in the Code_Aster model (or calculated based on elastic data in the case of pore compressibility) and (b) the final values estimated in model calibration (see Tab. 2-1). Three variations of input parameter distributions are considered, as described below and shown in Fig. 6-2.

Case 1A focuses on uncertainty of the bentonite materials over the range between the initial guesses that were calculated based on elastic data and the values estimated in model calibration (Fig. 6-2a). The resulting pressure profiles (Fig. 6-3) show low variation at early times, followed by a large uncertainty at later times (after 300 or 400 years). A histogram of the predicted maximum pressures is shown in Fig. 6-6a. As expected, the variation in maximum pressure predictions is low despite large variations in the bentonite properties. The mean value of the simulated maximum pressures and the maximum pressure simulated by the Code_Aster model are plotted for reference.

Uncertainty of the log pore compressibility at the distant formations (KEUK, AL, ML, DOGG, HERRE) and at the EDZ, which is assumed to be defined by the uniform pdfs shown in Fig. 6-2b, is considered in Case 1B. Somewhat significant increases in prediction uncertainty result, mostly near the maximum pressures at P14 and P17 (see Fig. 6-4 and Fig. 6-6b).

Case 1C considers uncertainty only in the two most influential parameters, the log pore compressibility and log pore expansivity of the host, which are given uniform pdfs over ranges between the values of the THM model and the values that were estimated in model calibration (Fig. 6-2b). As seen in Fig. 6-5, the vastly increased variation in simulated pressures, including in prediction of maximum pressures (Fig. 6-6c), highlights the relevance of these two parameters in the model abstraction process (i.e., the importance of estimating them accurately through model calibration).

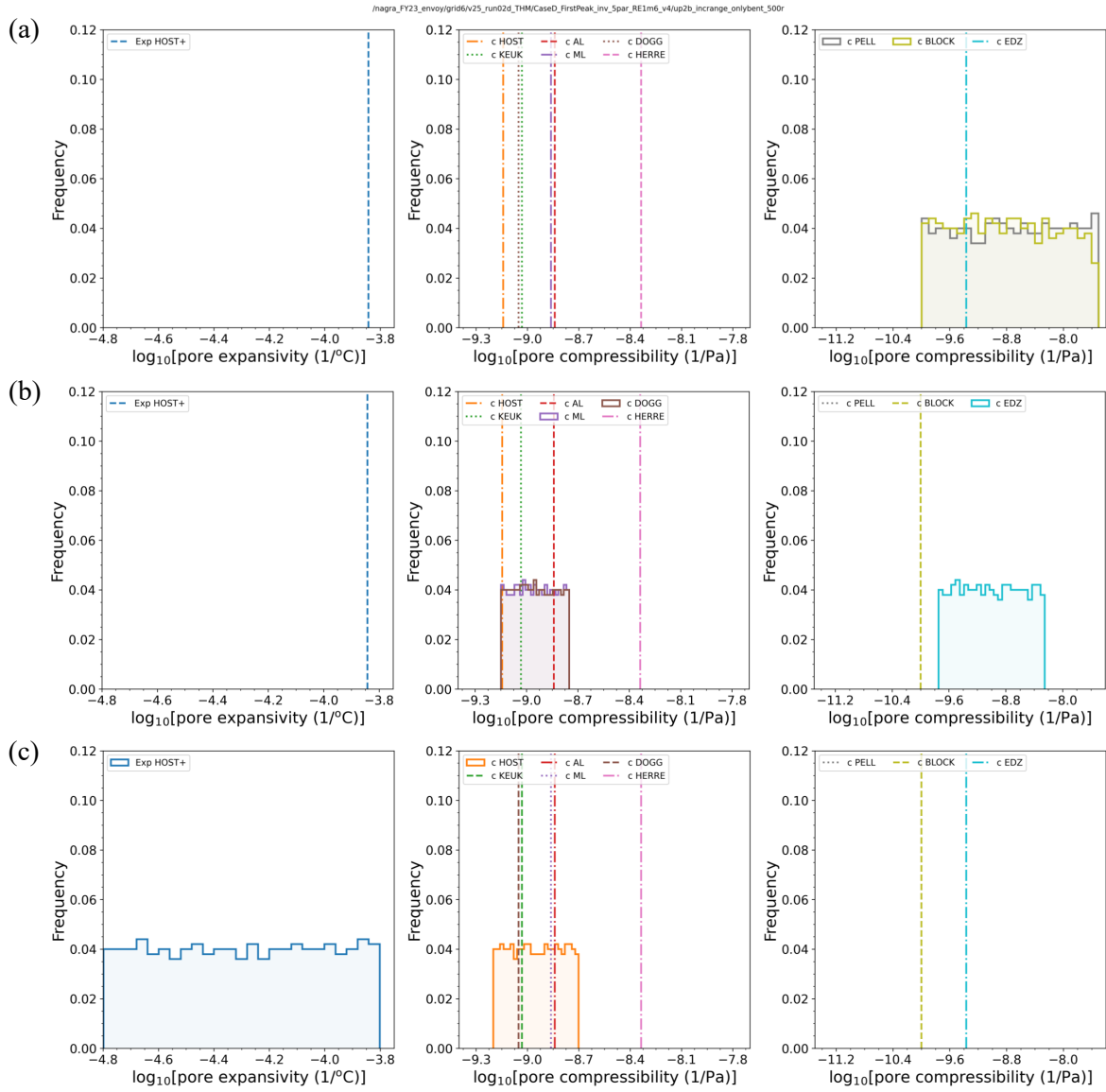


Fig. 6-2: Input parameter distributions for Analysis 1, with shaded polygons representing histograms of sampled parameters and vertical dashed lines indicating fixed parameter values

Different variations are considered in (a) Case 1A, (b) Case 1B, (c) Case 1C

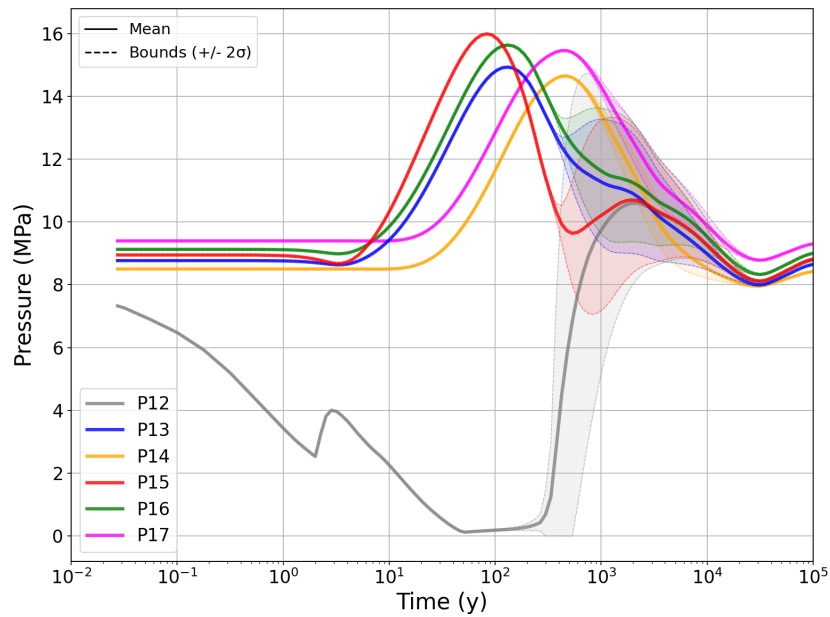


Fig. 6-3: Uncertainty of predicted time-series pressures for Case 1A, which assumes uniform uncertainty for bentonite pore compressibility values (see Fig. 6-2)

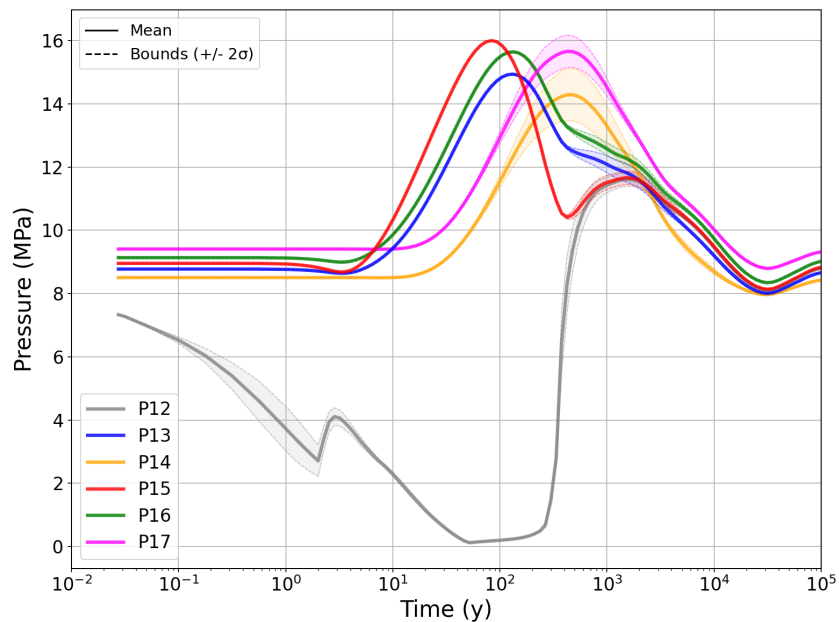


Fig. 6-4: Uncertainty of predicted time-series pressures for Case 1B, which assumes uniform uncertainty of the pore compressibility values of distant formations (see Fig. 6-2)

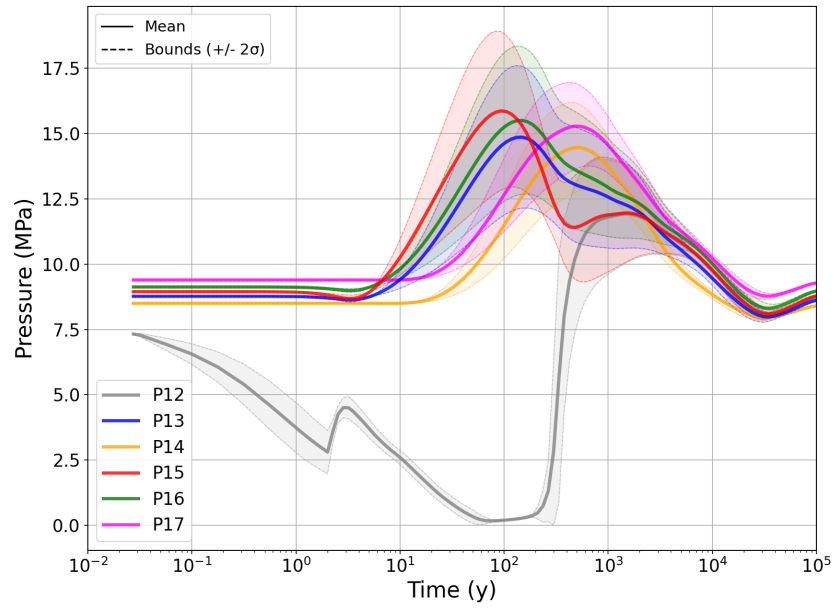


Fig. 6-5: Uncertainty of predicted time-series pressures for Case 1C, which assumes uniform uncertainty for pore expansivity and pore compressibility of host formation (see Fig. 6-2)

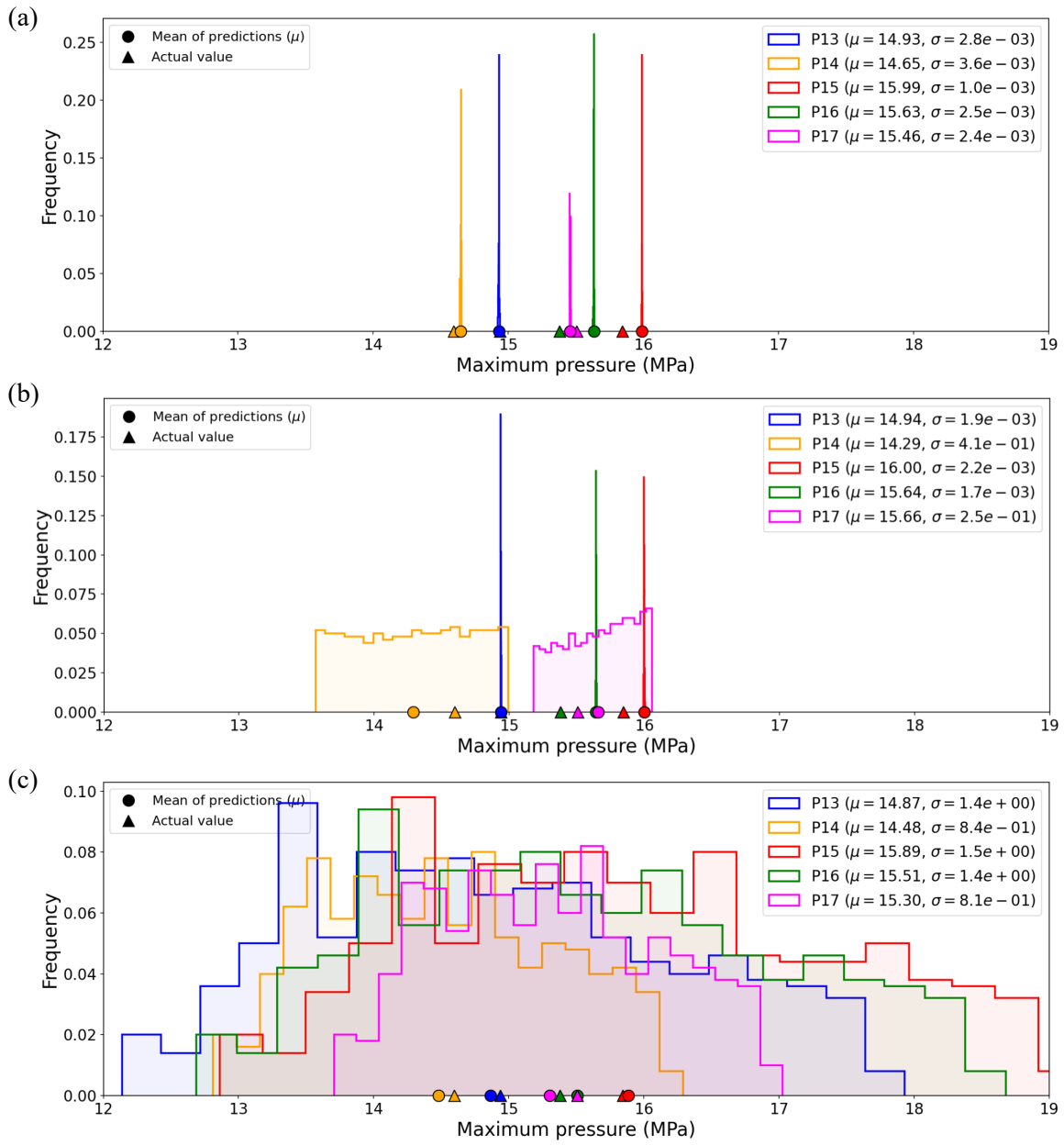


Fig. 6-6: Histograms of predicted maximum pressure for Cases (a) 1A, (b) 1B, and (c) 1C corresponding to respective input parameter distributions shown in (see Fig. 6-2)

6.3 Analysis 2 – Prediction uncertainty based on actual parameter estimation uncertainty, plus conservative variations

The analysis in this section is based on the actual (low) estimation uncertainty in the model abstraction process (i.e., the uncertainty of the parameter estimates), along with a few increasingly conservative variations. The histograms of input parameter values for each case are shown in Fig. 6-7.

The first case (Case 2A) uses the actual uncertainty distributions of the estimated parameters; that is, normal pdfs are defined by the means and standard deviations calculated based on a linearity and normality assumption (see Tab. 5-4, and Fig. 6-7a). These parameters include the HOST pore expansivity, and the pore compressibility for the formation materials (HOST, DOGG, and EDZ). The pore compressibility values of the bentonite materials (BLOCK and PELLE) are fixed (values shown by vertical dashed lines in Fig. 6-7a). The resulting prediction uncertainty in pressure is minimal, to the extent that the upper and lower bounds are hard to discern from the mean values in Fig. 6-8. As seen in Fig. 6-12a, the uncertainty in the prediction of maximum pressure is low, with an average standard deviation of 0.053 MPa. The means of the predicted maximum pressures (solid circles) are close to the actual pressures (solid triangles) as simulated by the Code_Aster model, although the iTOUGH2 predictions are slightly higher than the Code_Aster values at P15 and P16 (0.14 and 0.26 MPa, respectively).

The second and third cases (Cases 2B and 2C) are increasingly conservative in that they assume the standard deviations are larger by a factor of two and three, respectively, relative to their estimated values (see Fig. 6-7b and Fig. 6-7c). Uncertainty in the respective predicted pressure increases slightly (see Fig. 6-9 and Fig. 6-10), with average uncertainty in the predicted maximum pressures increasing (Fig. 6-12b and Fig. 6-12c), approximately linearly, to 0.11 MPa and 0.16 MPa.

The fourth case (Case 2D) increases the standard deviation of the parameter estimates significantly further, to a factor of five times the estimated value; in addition, this case incorporates potential uncertainty in the bentonite pore compressibility parameters (for demonstration purposes), assuming normal distributions with (1) the means centred between the values used in the Code_Aster simulation and the values assumed in the iTOUGH2 model calibration, and (2) exceedingly large standard deviations of 1.0 (see Fig. 6-7d). Accordingly, the uncertainty in the simulated pressures increases dramatically at later times due to the assumed bentonite uncertainty, which is not relevant for prediction of maximum pressures. Only a modest increase in predicted uncertainty of the maximum pressures is observed (Fig. 6-11), with average uncertainty in the predicted maximum pressures increasing to 0.26 MPa (Fig. 6-12c), due to uncertainty in the non-bentonite parameters (i.e., pore expansivity for HOST, and pore compressibility for HOST, EDZ, ML, and DOGG).

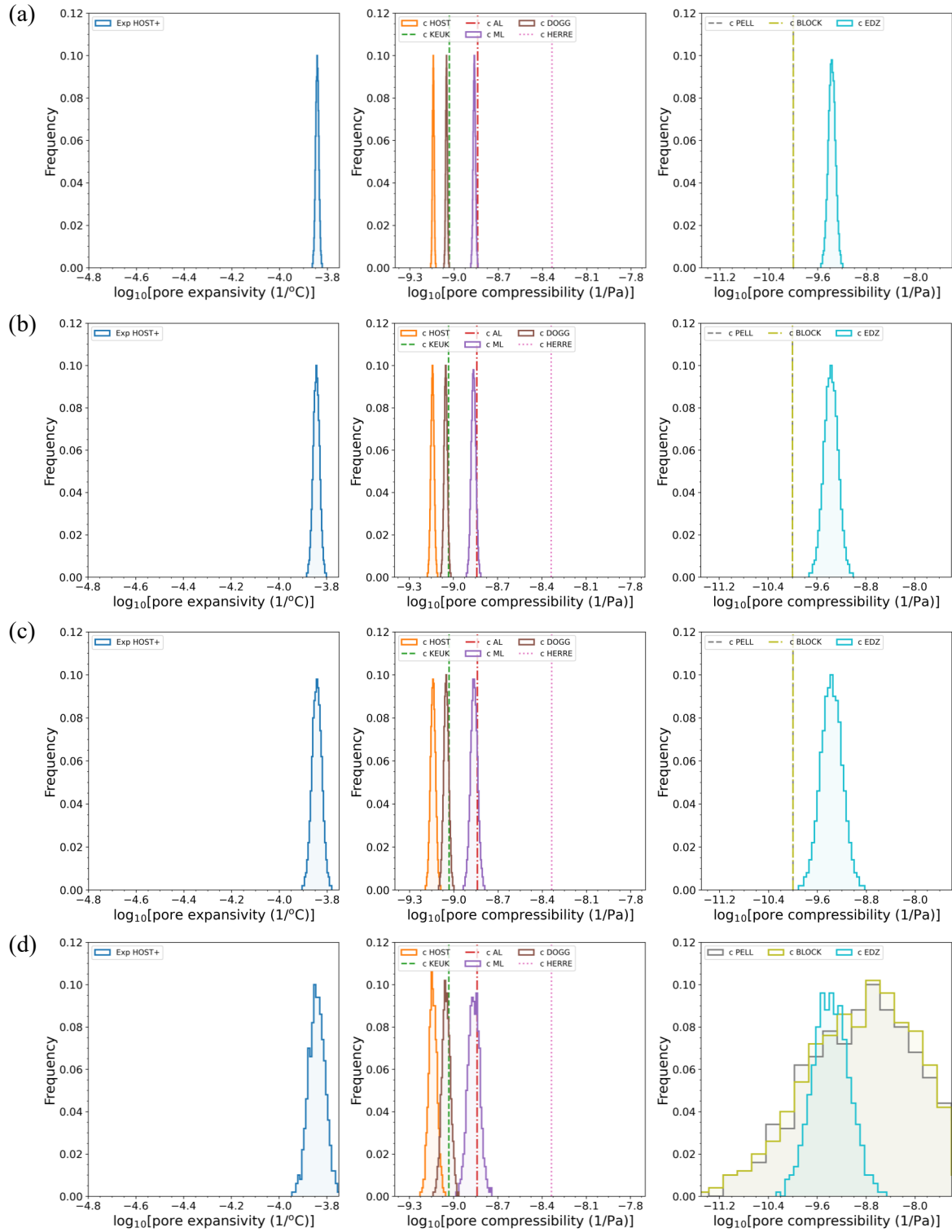


Fig. 6-7: Input parameter distributions for Analysis 2, with shaded polygons representing histograms of sampled parameters and vertical dashed lines indicating fixed parameter values

Different variations are considered in (a) Case 2A, (b) Case 2B, (c) Case 2C.

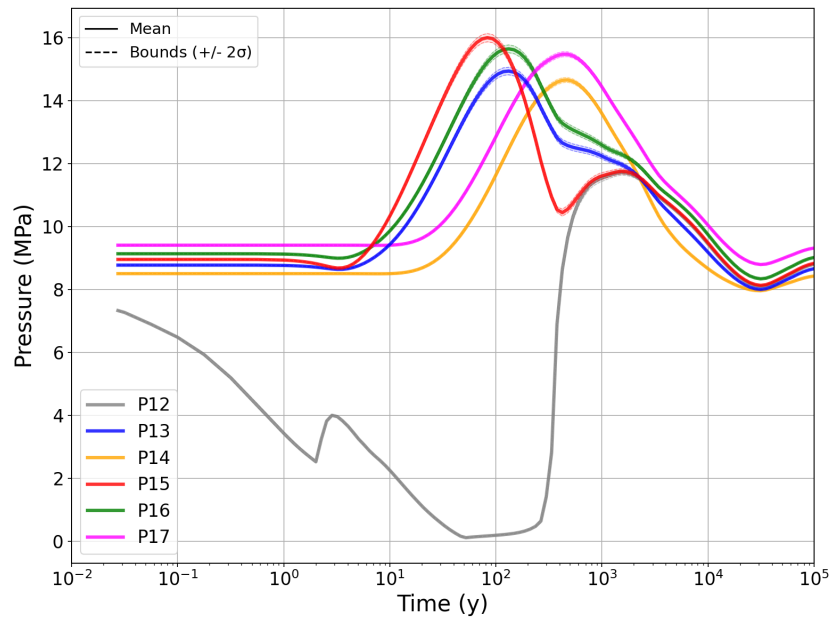


Fig. 6-8: Uncertainty of predicted time-series pressures for Case 2A based on input parameter distributions that are estimated by model calibration
(Fig. 6-7a)

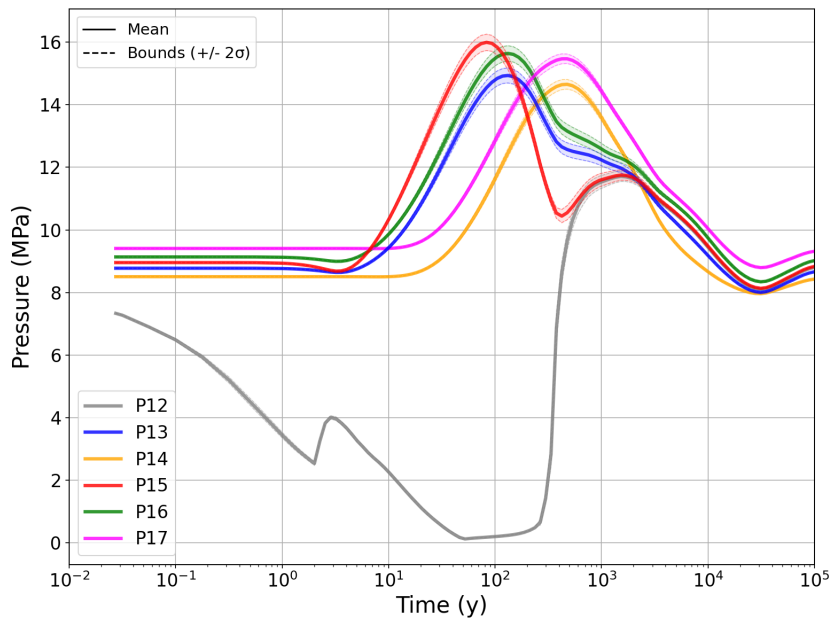


Fig. 6-9: Uncertainty of predicted time-series pressures for Case 2B, which is similar to Case 2A, except uncertainty in the input parameter distributions is increased by a factor of 2.0 over what was estimated in model calibration
(see Fig. 6-7b)

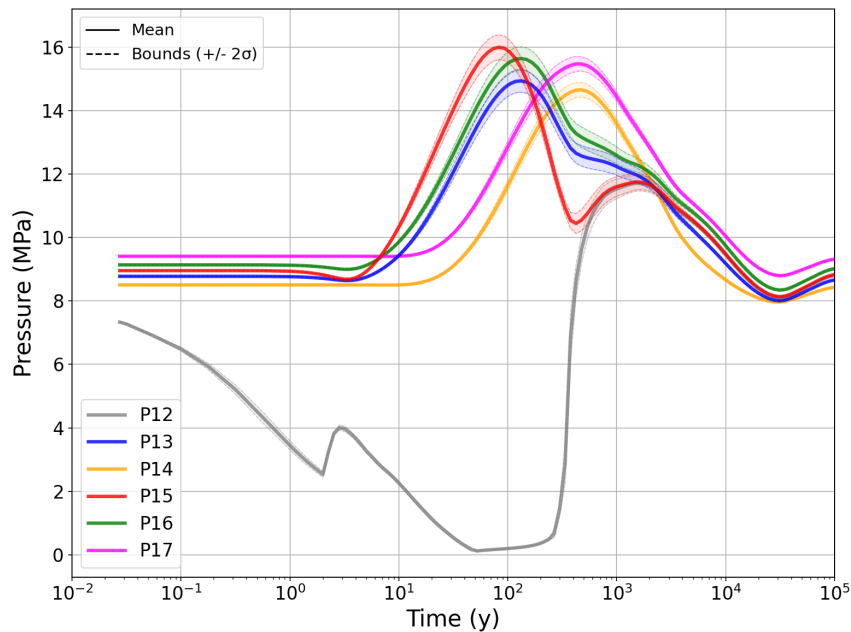


Fig. 6-10: Uncertainty of predicted time-series pressures for Case 2C, which is similar to Case 2A, except uncertainty in the input parameter distributions is increased by a factor of 3.0 over what was estimated in model calibration

(see Fig. 6-7c)

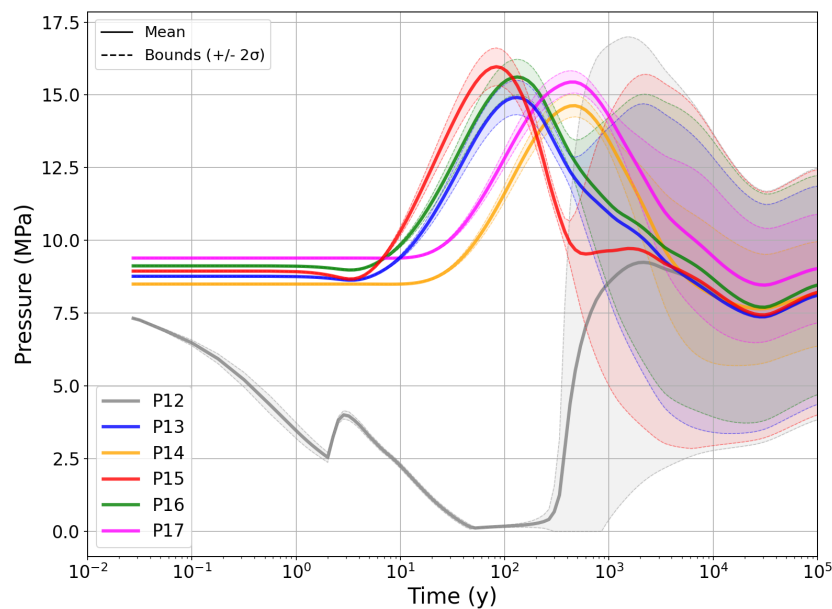


Fig. 6-11: Uncertainty of predicted time-series pressures for Case 2D, which is similar to Case 2A, except that uncertainty in the input parameter distributions is increased by a factor of 5.0 over what was estimated in model calibration, and exaggerated uncertainty in the bentonite parameters is introduced for demonstration purposes

(see Fig. 6-7d)

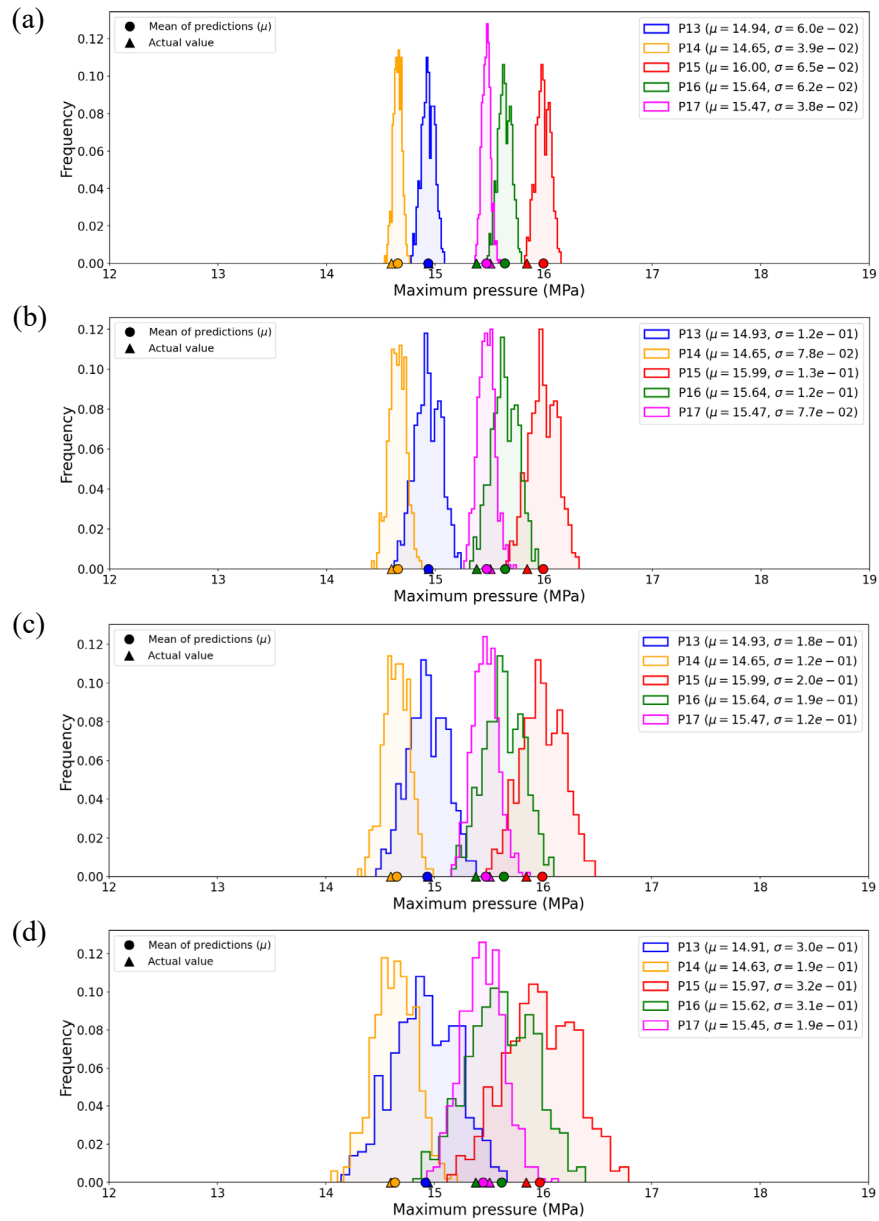


Fig. 6-12: Histograms of predicted maximum pressure for Cases (a) 2A, (b) 2B, (c) 2C, and (d) 2D

6.4 Analysis 3 – Prediction uncertainty due to overall model uncertainty (example with formation permeability)

The final, third analysis demonstrates the impact of overall model uncertainty that is expected to be relevant – not in the model abstraction step, but in general applications of the model, where additional sources of model uncertainty exist (e.g., uncertainty in permeability of geological formations). It is expected that such model uncertainty will influence prediction uncertainty more than that originating in the model abstraction step alone.

To demonstrate this point, four cases with increasing levels of uncertainty in the log permeability are considered. The probability distributions are described in Tab. 6-1 and shown in Fig. 6-13.

In this first case (Case 3A), an overly optimistic low level of uncertainty ($\sigma = 0.05$ [$\log_{10}(k(m^2))$]) for log permeability is specified in the input parameter distributions for relevant geological formations; the uncertainty distributions are defined by normal distributions with the means set to the true values (i.e., the values that the Code_Aster and iTOUGH2 models use), as shown in Fig. 6-13a. An overall increase in uncertainty of the predicted pressures (Fig. 6-14) and the maximum pressures is seen, with the uncertainty in the maximum pressure given by an average standard deviation of 0.13 MPa, which is (a) around 2.5 times larger than the average uncertainty for predictions made with the base-case calibrated model (Case 2A), which was 0.053 MPa. The largest average prediction uncertainty prediction uncertainty with the calibrated model was 0.26 MPa for Case 2D, but that was the most conservative case for which assumed estimation uncertainty was 5 times larger than what was inferred by model calibration.

When the standard deviation of the input log permeability distributions increases to more reasonable values of 0.1, 0.2, and 0.3, the average estimation uncertainty of maximum pressure increases dramatically to 0.26, 0.52, and 0.74 MPa. The corresponding prediction uncertainty for pressure profiles is shown in Fig. 6-15, Fig. 6-16, and Fig. 6-17, respectively. And the histograms of maximum pressure predictions and corresponding uncertainty measures are shown in Fig. 6-18.

Tab. 6-1: Probability distribution of uncertain input parameters for Analysis 3

Parameter	Material	Mean	Std. dev. [σ]	Lower bound	Upper bound
$\log_{10}(\text{permeability (m}^2\text{)})$	HOST	-21.04		-22.0	-18.0
	EDZ	-21.04	Case 3A (0.05)	-22.0	-18.0
	KEUK	-20.74	Case 3B (0.1)	-22.0	-18.0
	AL	-20.74	Case 3C (0.2)	-22.0	-18.0
	ML	-20.34	Case 3D (0.3)	-22.0	-18.0
	HERRE	-19.04		-22.0	-18.0
	DOGG	-20.65		-22.0	-18.0

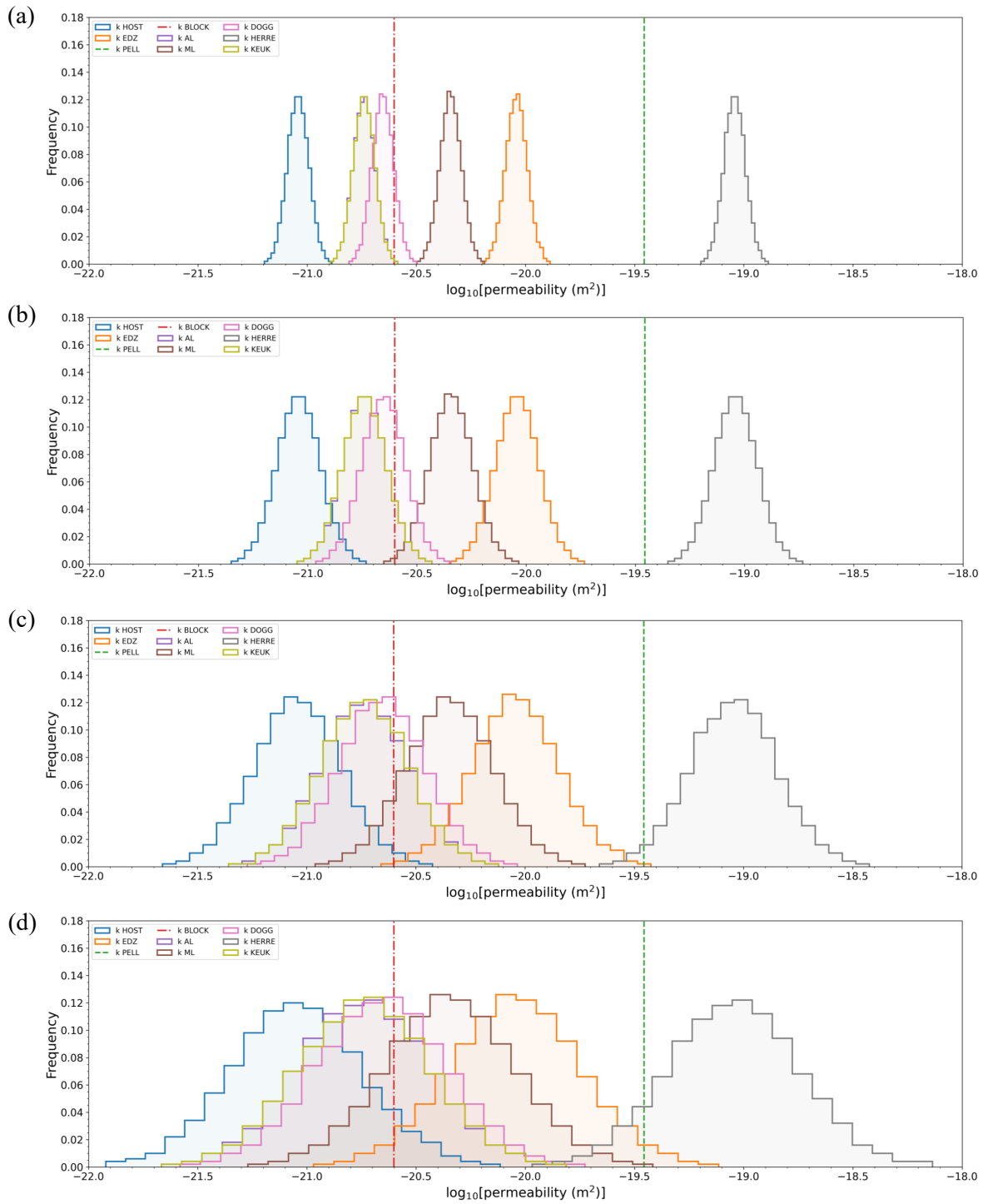


Fig. 6-13: Log permeability distributions for Analysis 3, with increasing standard deviations
 (a) Case A, $\sigma = 0.05$; (b) Case 3B, $\sigma = 0.1$, (c) Case 3C, $\sigma = 0.2$, and (d) Case 3d, $\sigma = 0.3$,
 in units of $\log_{10}[(\text{m}^2)]$

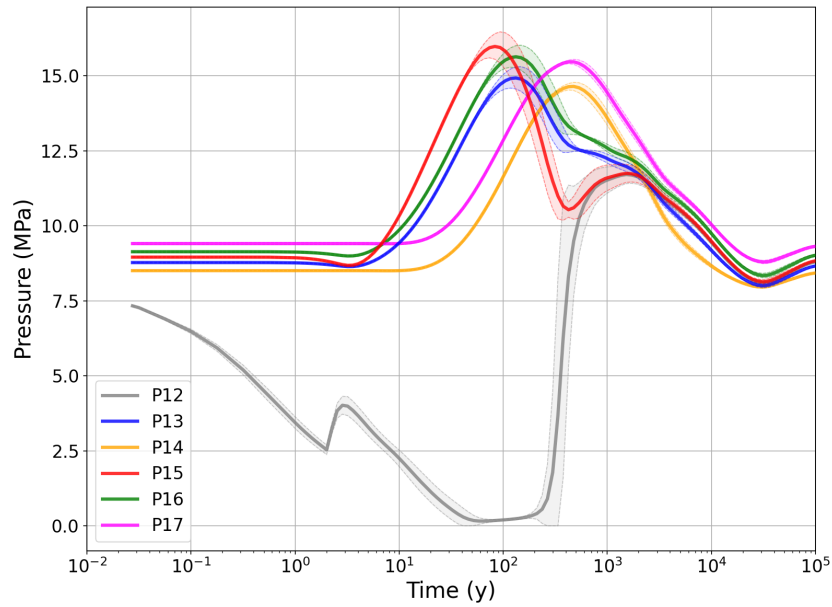


Fig. 6-14: Uncertainty of predicted time-series pressures for Case 3A, which assumes $\sigma = 0.05$ for the normal distributions of log permeability input parameters (Fig. 6-13a)

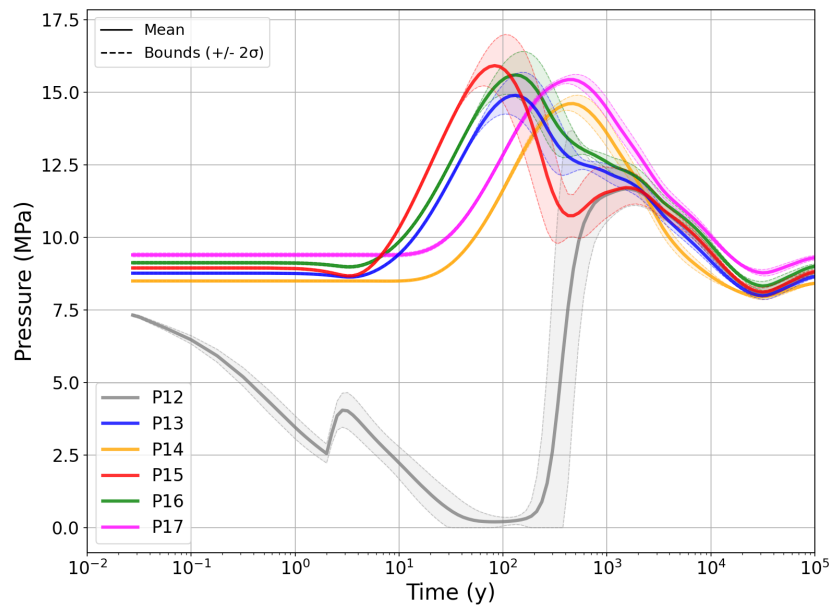


Fig. 6-15: Uncertainty of predicted time-series pressures for Case 3A, which assumes $\sigma = 0.1$ for the normal distributions of log permeability input parameters (Fig. 6-13b)

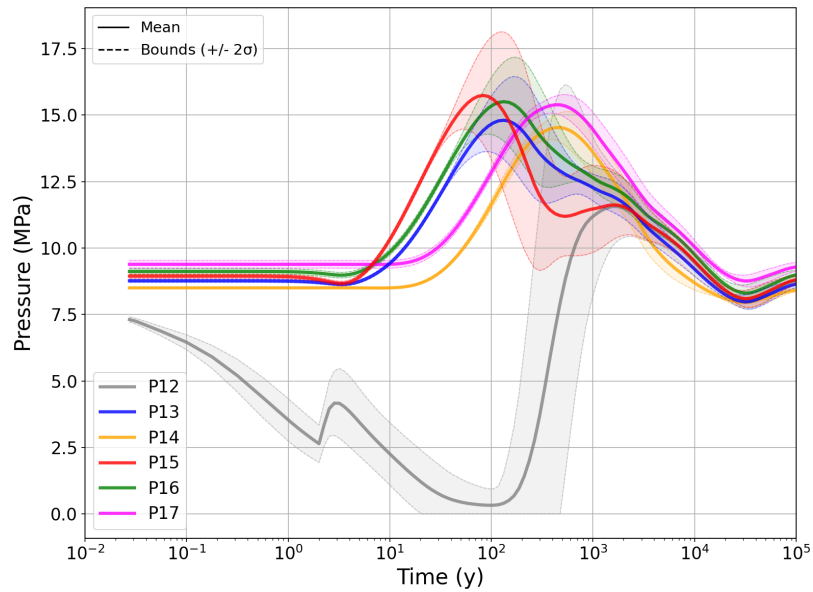


Fig. 6-16: Uncertainty of predicted time-series pressures for Case 3A, which assumes $\sigma = 0.2$ for the normal distributions of log permeability input parameters (Fig. 6-13c)

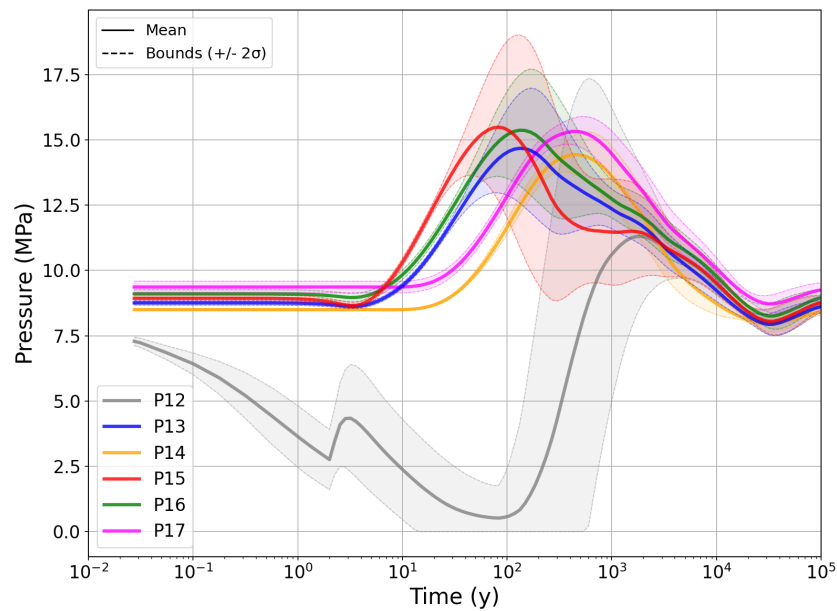


Fig. 6-17: Uncertainty of predicted pressure series for Case 3C, which assumes $\sigma = 0.3$ for the normal distributions of log permeability input parameters (Fig. 6-13d)

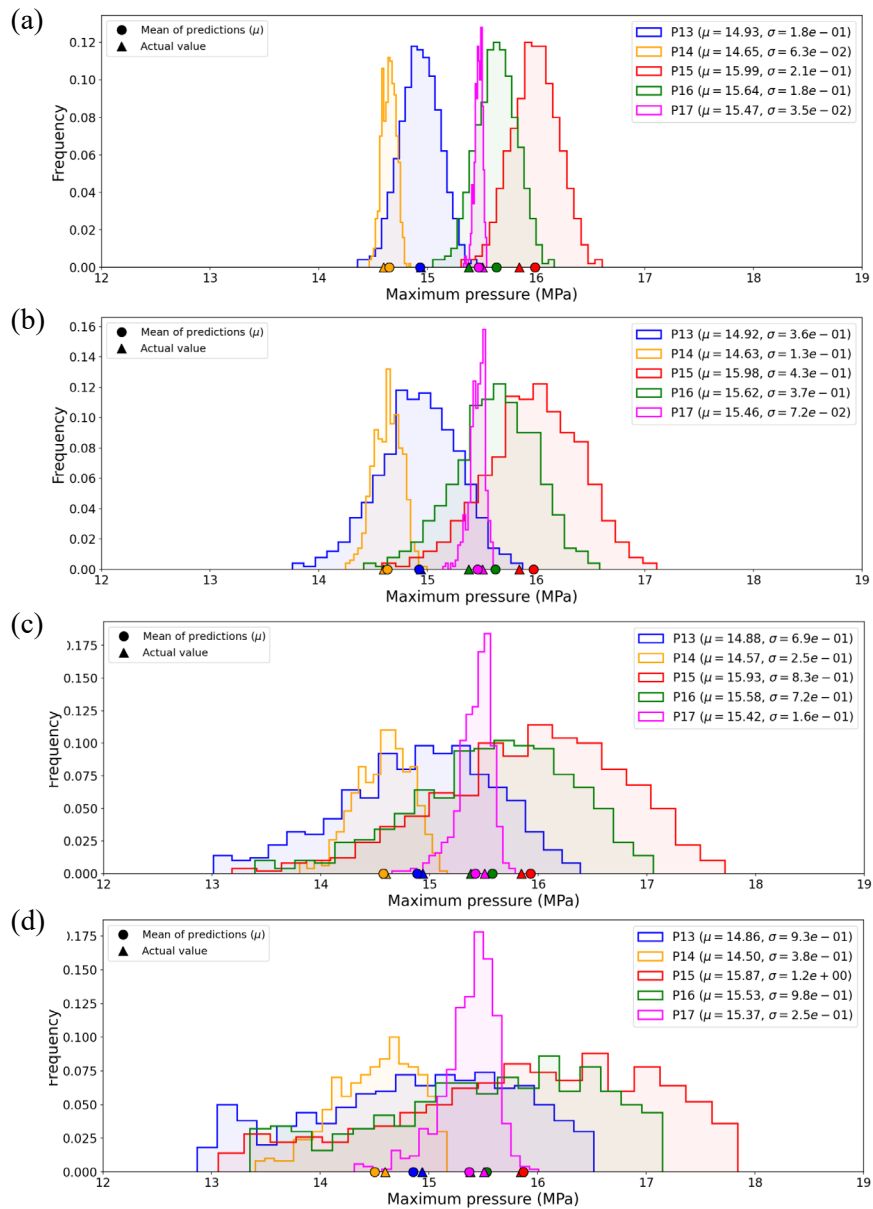


Fig. 6-18: Histograms of predicted maximum pressure for Cases (a) 3A, (b) 3B, (c) 3C, and (d) 3D

Based on the respective normal distributions of log permeability input parameters shown in Fig. 6-13

7 Total stress analysis

7.1 Approach

A semi-analytical approximation of stress evolution near the canister within the bentonite buffer was recently developed by Lengler et al. (personal communication) for Nagra candidate sites, providing an efficient way to estimate mechanical effects based solely on post-processing of simulation output from TH simulations (i.e., without requiring computationally intensive, fully coupled THM simulations to account for stress conditions and nonlinear behaviour of bentonite swelling). Lengler et al. (pers. communication) validated the approach by comparing the semi-analytical solution to results obtained with the fully coupled THM simulator Code_Aster, providing confidence that this approximation can be used – together with simulation output from the calibrated TH model obtained through the THM-TH abstraction process in this study (see Section 5.3.1) – to examine stress build-up due to bentonite swelling and the subsequent changes in stress in response to evolving pore pressures after the bentonite becomes fully liquid saturated, accounting for the compressibility and thermal expansion or contraction of the pore space.

The approach decomposes the evolution of incremental total mean stress into two phases (before and after the bentonite is fully hydrated) with separate sets of equations, as follows:

(1) The swelling phase during the hydration phase of the bentonite, based on a nonlinear elastic swelling constitutive framework (Gérard et al. 2008):

$$d\sigma_{T,t} = B \cdot dp_{g,t} + dp_{s,t} \quad (1)$$

with

$$dp_{s,t} = A \cdot B \cdot \left(\frac{\sqrt{\pi}}{2\sqrt{\beta}} \left[\text{Erf} \left(\frac{p_{c,t}}{A} \sqrt{\beta} \right) - \text{Erf} \left(\frac{p_{c,t-1}}{A} \sqrt{\beta} \right) \right] - \frac{1}{2\beta} \left[e^{-\beta \left(\frac{p_{c,t}}{A} \right)^2} - e^{-\beta \left(\frac{p_{c,t-1}}{A} \right)^2} \right] \right) \quad (2)$$

$$B = 1 - \frac{K}{K_s} \quad (3)$$

where $d\sigma_{T,t}$ is the change in total mean stress and $dp_{g,t}$ is the change in gas pressure at time step t from the previous time step, i.e., $dp_{g,t} = p_{g,t} - p_{g,t-1}$. The change in swelling pressure $dp_{s,t}$ is a function of the (positive) capillary pressures $p_{c,t}$ and $p_{c,t-1}$, at the current time step and the previous time step, respectively, and A is a reference pressure (with the same units as p_c and p_g). The swelling parameter β (unitless) is a swelling model parameter that is related to the maximum swelling pressure. K and K_s are the bulk moduli (Pa) of the porous medium and solid skeleton, respectively.

(2) The post-swelling phase, after the bentonite becomes fully liquid-saturated, with thermo-poro-elastic effects:

$$d\sigma_{T,t} = B \cdot dp_t - K \cdot \frac{\varphi_t - \varphi_0}{B - \varphi_0} + K \cdot \frac{\varphi_0 \alpha_T}{1 - \varphi_0} \cdot (T_t - T_0) \quad (4)$$

where dp_t is the change in pressure, at time step t , relative to the previous time step, φ_t and φ_0 are the porosities at time step t and the initial porosity, respectively, α_T is the thermal expansion coefficient (1/K), and T_t and T_0 (°C) are the temperatures at time step t and the initial temperature, respectively.

7.2 Analysis 1 – Estimated stress for calibrated TH model

Total stress evolution is estimated using the semi-empirical approach with simulation output from the calibrated TH model of this study; the results are shown in Fig. 7-1. The input parameters include a maximum swelling pressure of 4 MPa, which corresponds to the expected bentonite density, and $A = 1$ MPa, yielding a β value of 0.232. The bulk moduli of the bentonite pedestal and buffer are 0.167 GPa and 0.103 GPa, respectively, while α_T is 2.5×10^{-5} 1/K. K_s is assumed to be infinite, making $B = 1.0$.

For the swelling phase (Fig. 7-1a), the stresses increase at a similar rate at each control point, to around 4 MPa. In the post-swelling phase (Fig. 7-1b), after the bentonite is fully saturated, the stresses continue to build, to maximum values of approximately 13 MPa around the same time at each control point, between 1,400 and 1,500 years, which corresponds to the time when maximum pressures were reached in the bentonite materials (see Fig. 3-6) and when the temperatures had already started to decrease (Fig. 3-7). The stresses are slightly higher (less than 0.5 MPa higher) in the bentonite buffer (P2 through P6) than in the pedestal (P7 through P9).

7.3 Analysis 2 – Sensitivity of estimated stress to bentonite properties

The sensitivity of the total stress to bentonite material properties, which serve as input parameters to the semi-analytical stress approximation (Section 7.1), is demonstrated in Fig. 7-2 through Fig. 7-5.

Increasing the maximum swelling pressure increases the maximum stress in the swelling phase to around 7 MPa (Fig. 7-2a), as expected, and to around 16 MPa in the post-swelling phase (Fig. 7-2b). It is also interesting to note that the stress increase at P9 in the swelling phase begins earlier than for the other control points (Fig. 7-2a) because the water saturation increases relatively earlier at this location (e.g., see Fig. 3-8).

Sensitivity of the total stress to the thermal expansivity is demonstrated in Fig. 7-3, to which only the post-swelling phase stress evolution is expected to be sensitive. With the decreased value of α_T , the stress increases slightly toward the end of the simulation (relative to the base case in Fig. 7-1b) at most of the control points, whereas the total stress at P6 and P9 decreases slightly at around 1,500 years (relative to the base case in Fig. 7-1b). Although the differences are subtle, this example illustrates how contributions from different terms in the post-swelling stress equations impact different portions of the stress time series, reflecting complex thermo-hydromechanical effects.

Lastly, the sensitivity of the total stress to the bulk modulus of the bentonite is illustrated in Fig. 7-4 and Fig. 7-5, with values increased (multiplied by 2.0) and decreased (multiplied by 0.5), respectively. The corresponding maximum stress values are seen to vary considerably in the post-swelling phase (Fig. 7-4b and Fig. 7-5b), with differences between the cases of over 0.5 MPa.

It is obvious that the calculated total stresses are not only uncertain due to uncertainties in the geomechanical parameters investigated here, i.e., maximum swelling pressure, thermal expansivity, and bulk modulus; they are also influenced by the uncertainties in the predicted pore pressures, as discussed in Section 6 above.

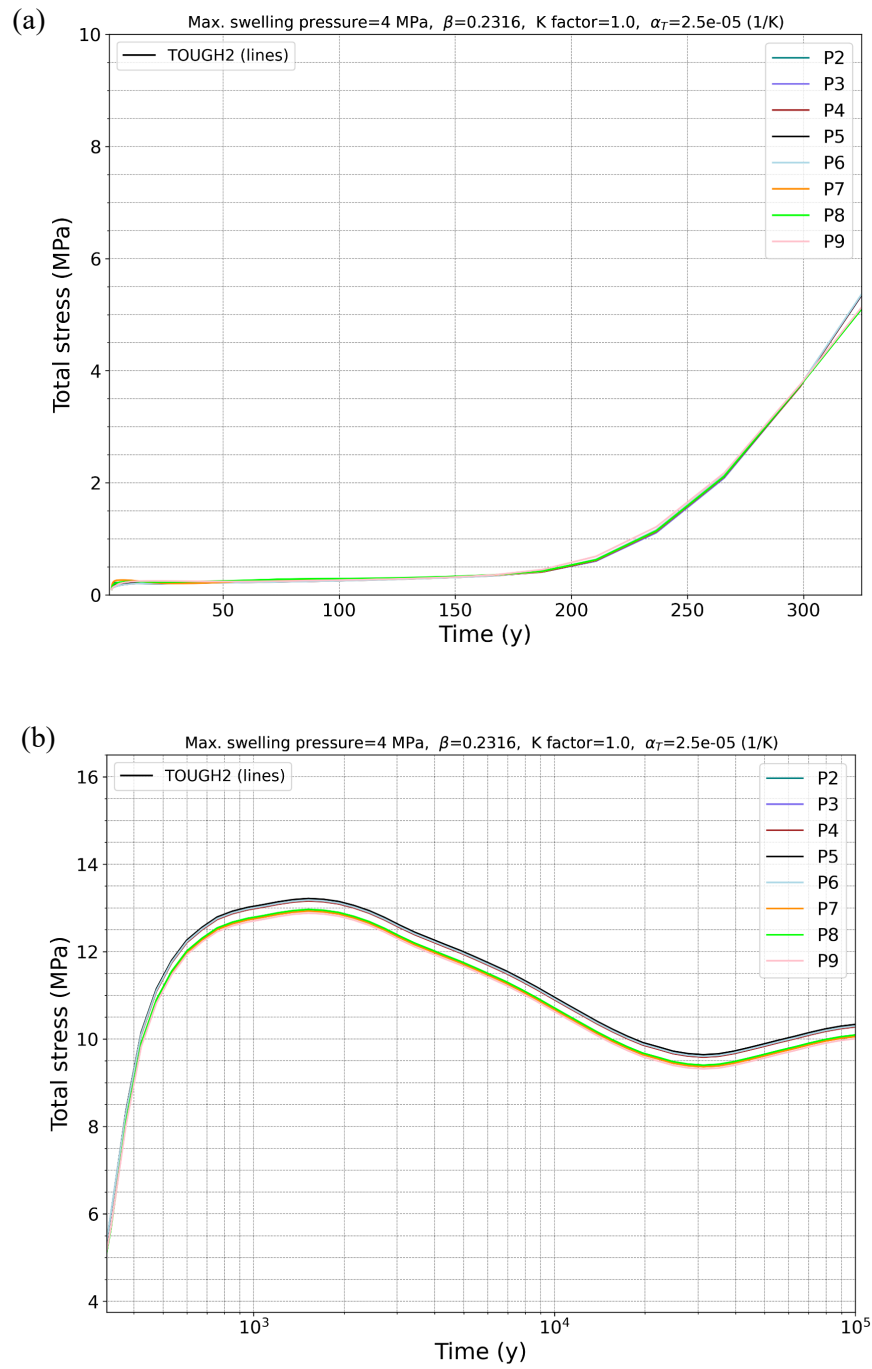


Fig. 7-1: Semi-analytical approximation of the stress evolution at control points P2 through P9, based on TH simulation output

(a) swelling phase and (b) post-swelling phase

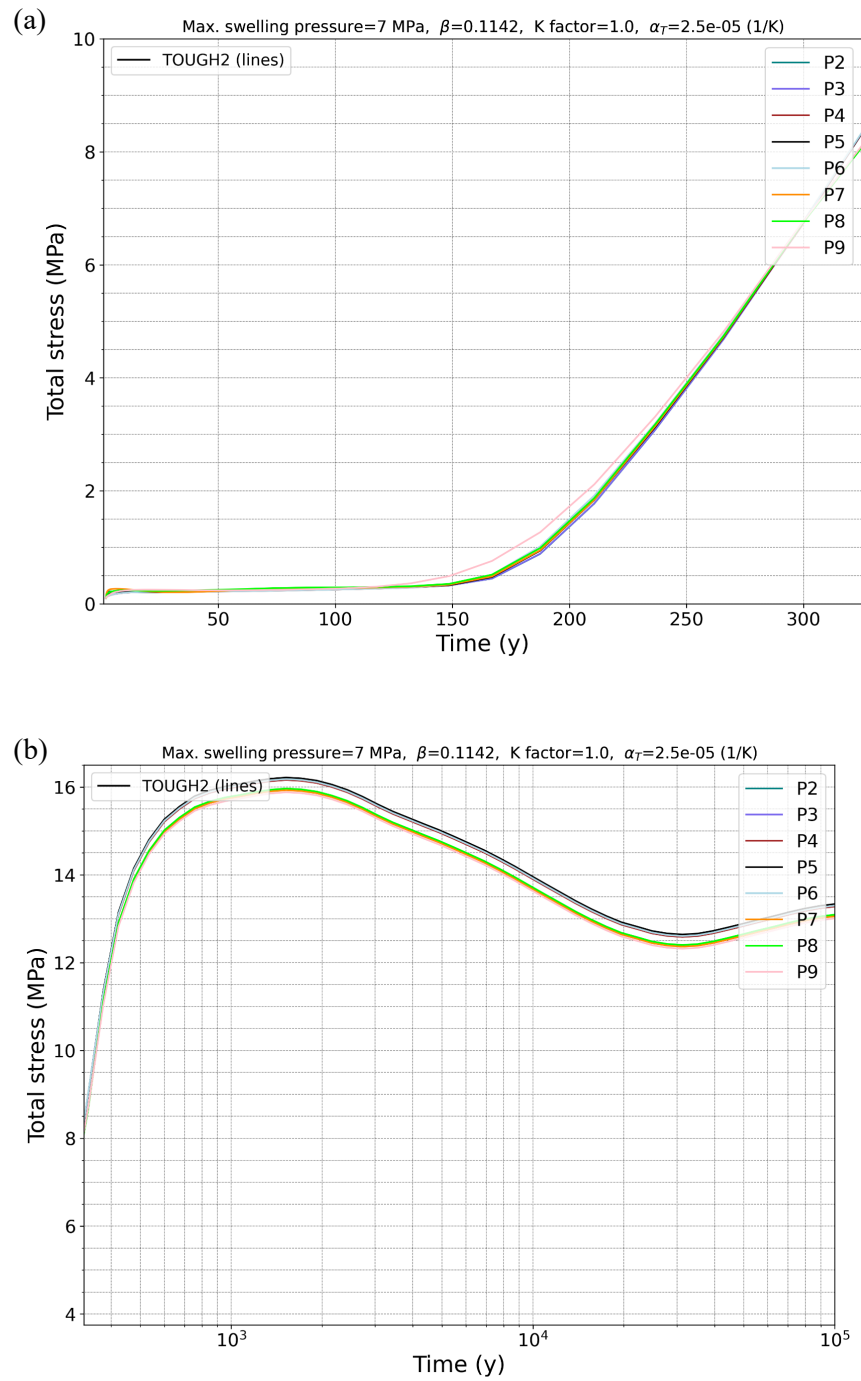


Fig. 7-2: Total stress with maximum swelling pressure increased to 7 MPa. Semi-analytical approximation of the stress evolution at control points P2 through P9, based on TH simulation output

(a) swelling phase and (b) post-swelling phase

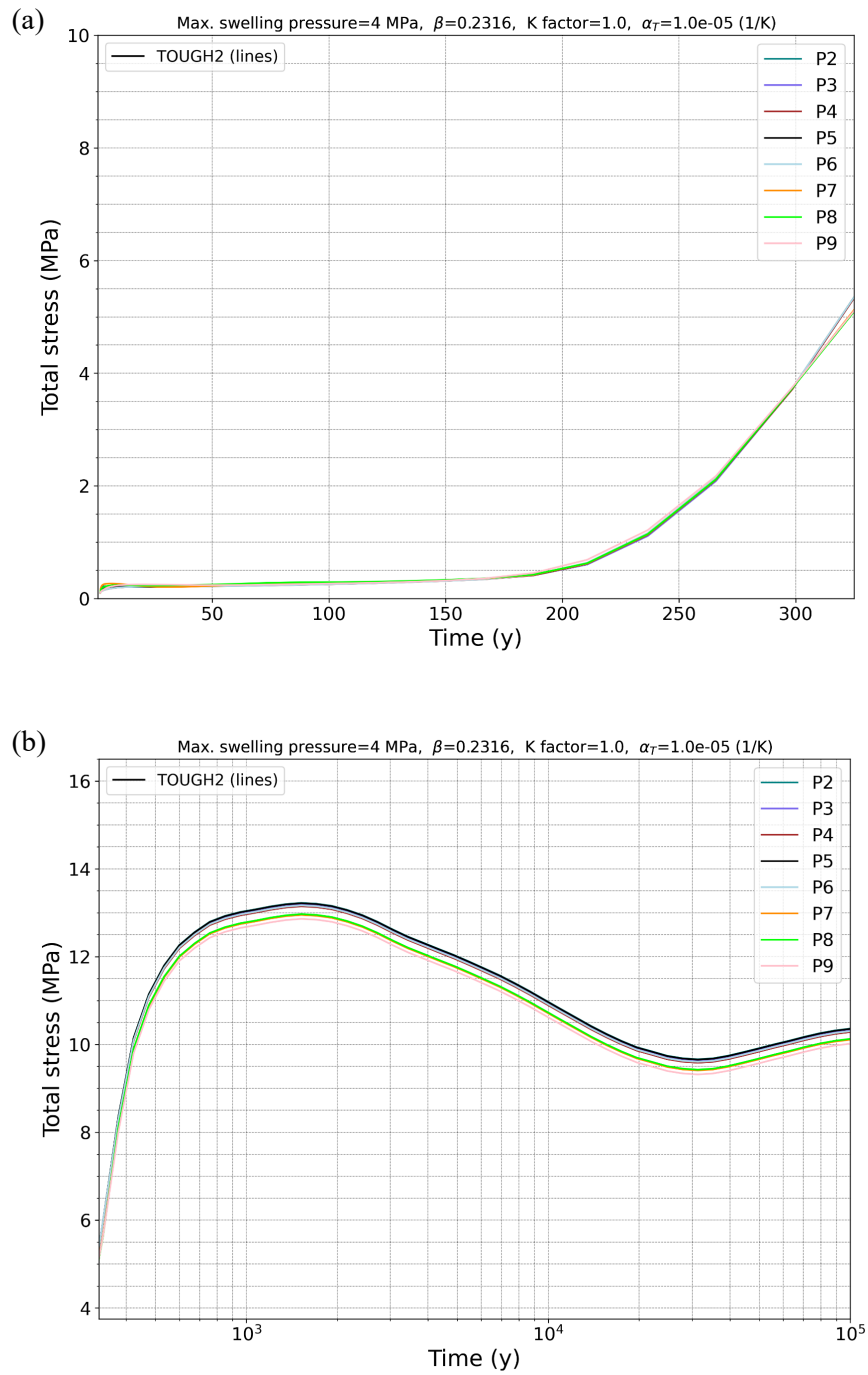


Fig. 7-3: Total stress with thermal expansivity decreased to 10^{-5} K^{-1} . Semi-analytical approximation of the stress evolution at control points P2 through P9, based on TH simulation output

(a) swelling phase and (b) post-swelling

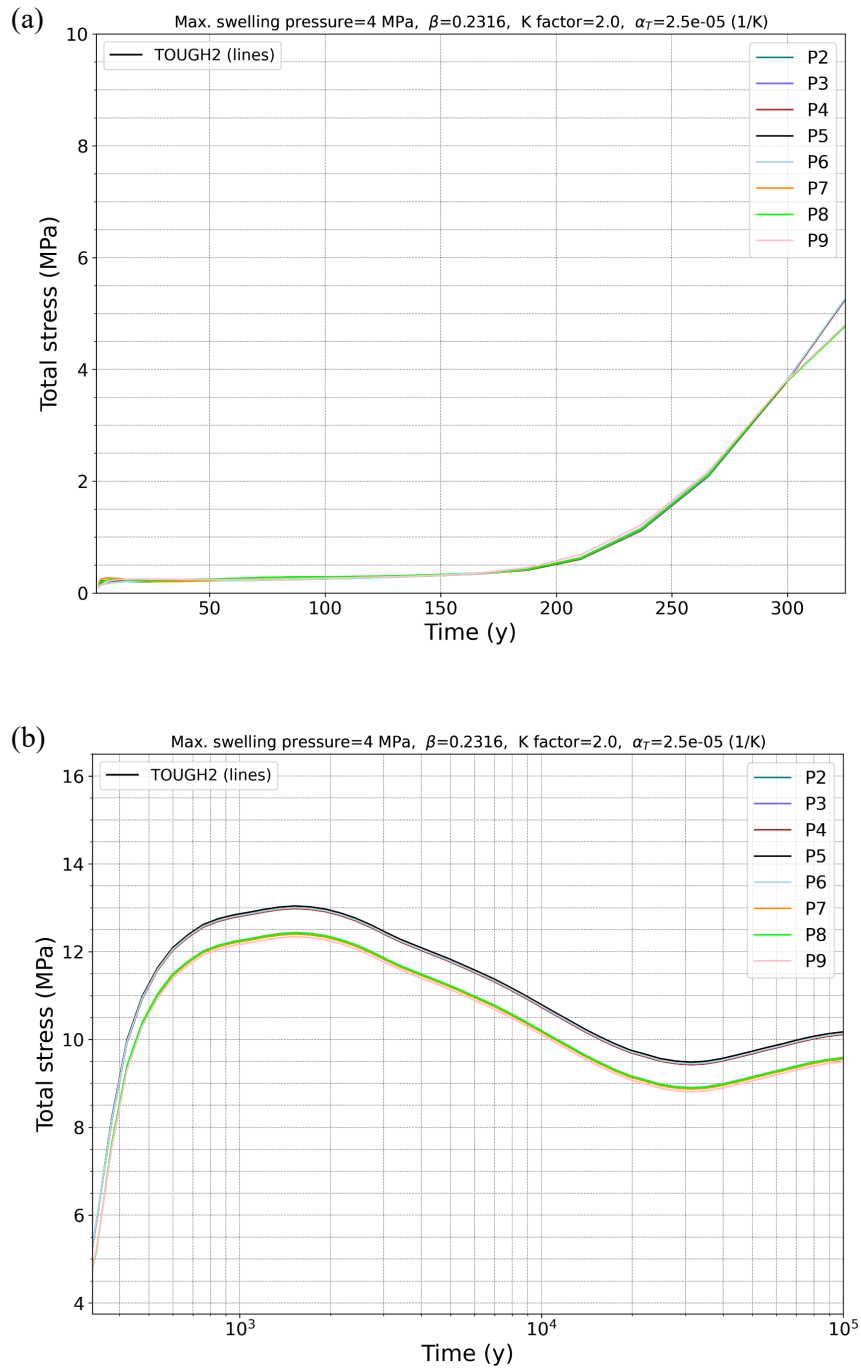


Fig. 7-4: Total stress with bulk modulus increased (multiple by 2.0). Semi-analytical approximation of the stress evolution at control points P2 through P9, based on TH simulation output

(a) swelling phase and (b) post-swelling phase

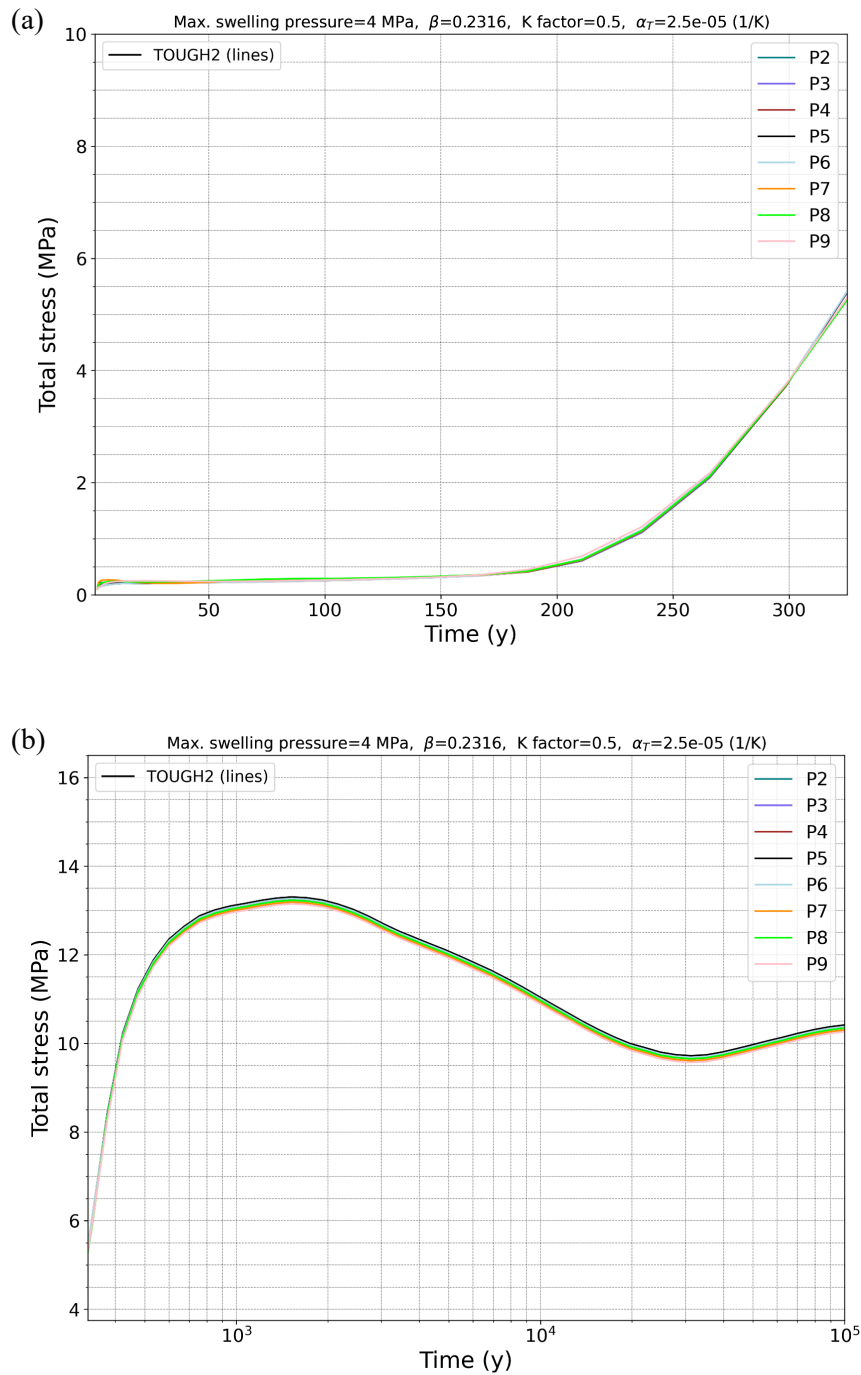


Fig. 7-5: Total stress with decreased bulk modulus (multiplied by 0.5). Semi-analytical approximation of the stress evolution at control points P2 through P9, based on TH simulation output

(a) swelling phase and (b) post-swelling phase

8 Summary and conclusions

An iTOUGH2-based numerical model was developed to simulate the behaviour in an HLW nearfield, based on the latest design for a repository disposal tunnel at the Nördlich Lägern site. More specifically, a TH prediction model is developed with specially determined volumetric deformation parameters, allowing for predictions of key processes to be made with accuracy that is comparable to predictions made by a high-fidelity, computationally demanding numerical model that accounts for coupled two-phase flow and mechanical effects, performed with Code_Aster (EDF 2024). The iTOUGH2 TH model is developed in a model-abstraction process that estimates a limited number of effective input parameters – corresponding to pore expansivity and/or pore compressibility for a limited number of materials in the EBS and surrounding geological formations. These parameters are estimated through inverse modelling, using synthetic data generated by the Code_Aster THM model at representative locations within the EBS, in the EDZ, and at distant points in the Opalinus Clay.

The complex simulation procedure involves a series of phases with intricate changes to initial and boundary conditions and material assignments, including (1) an equilibration phase, which simulates the near-steady-state profile that develops over a long time scale leading up to the present; (2) a short excavation (pre-ventilation) phase, which accounts for pressure changes in the system as the excavation nears the model domain; (3) a two-year ventilation phase, which begins after the tunnel is excavated and is opened to the atmosphere and the concrete liner is installed; and (4) a post-closure heating phase that starts when, simultaneously, the tunnel components (pedestal and bentonite buffer, and waste canister) are installed, the tunnel is sealed from the atmosphere, and the heating begins, which is the final phase that lasts for 100,000 years.

In the process of developing the iTOUGH2 model, simulated pressures, temperatures, saturations, and porosity values were compared – starting with comparisons between the output from the iTOUGH2 model and a TH version of the Code_Aster model, which allowed for identification and elimination of model inconsistencies that were not related to mechanical effects. Since both TH models should theoretically yield the same predictions, this exercise allowed for small adjustments to be made to each model, in an iterative fashion, to make them as consistent with each other as possible. The causes of some inconsistencies were not yet identified and are left for future work. For example, simulated maximum pressures were higher in the TH model than in the THM model, which is hypothesized to result from differences in how the flow of gas is handled between iTOUGH2 and Code_Aster.

Subsequently, synthetic data were generated by the THM version of the Code_Aster model to be used for estimation of the effective parameters in iTOUGH2 model calibration. An initial comparison of the Code_Aster THM results with the TH model output provides a first indication of the influence of mechanical effects on the predicted pressure distribution in the Opalinus Clay; it is this influence that needs to be captured by the iTOUGH2 TH model using the proposed abstraction methodology. It should be noted that setting pore compressibility of the bentonite materials to lower values allowed for an improved fit to the data.

In sensitivity analyses, it was observed that the sensitivity of pressure data to various parameters is affected by the assumed reference values. In one case that was based on initially assumed/calculated parameter values, the late-time pressure data were sensitive to the pore compressibility of bentonite materials; in a second case, based on parameter reference values that were close to those obtained through the model calibration, the late-time pressure showed higher sensitivity to pore expansivity than to bentonite properties. In any case, the early-time pressure data, which included the maximum pressures of interest, were highly sensitive to the pore expansivity and pore compressibility of the host rock, and the permeability of the host rock (along with other parameters, depending on the location of the observation). In general, the sensitivity of later-time

pressures was complicated by uncertainty in the representation of the bentonite materials in the tunnel and late-arriving pressure-wave reflections. Therefore, a subset of pressure data from earlier times was selected for use in model calibration, along with temperature data from all times.

The simulated predictions of interest in this study, namely the pressure response, have low sensitivity to the absolute value of the initial porosity, but it is expected that minor variations in the function that relates changes in effective pressures and saturation to changes in porosity has a significant effect on pressure predictions.

A base-case inversion of time-series pressures and temperatures was performed, resulting in a model that serves as the basis for subsequent uncertainty propagation analysis. The sensitivity of inversion results to the weight assigned to synthetic data at the control point (P12) in the EDZ was also examined, as was the use of maximum pressures (instead of time series pressure) for model calibration. Even for the best-case scenario of inversion using maximum pressures, a higher degree of parameter correlation and overall worse results are observed than for the base-case inversion that uses time-series pressures.

Inspection of the objective function of the base-case inversion shows that despite non-uniqueness in the inverse solution due to correlation between the pore compressibility and pore expansivity, the synthetic data are sufficiently sensitive to obtain a unique solution with low estimation uncertainty. In general, inversion of the Code_Aster THM synthetic data resulted in parameter estimates with low estimation uncertainty and with low residuals, yielding a calibrated iTOUGH2 model that could be used to predict maximum pressures with acceptable accuracy.

Finally, the impact of potential sources of uncertainty in the iTOUGH2 model on predictions of interest was evaluated through Monte Carlo simulations with Latin Hypercube Sampling. The primary goal, which was to obtain an abstracted iTOUGH2 TH model that could effectively predict the maximum pressures in the Opalinus Clay, was achieved. The impact of overall model uncertainty, such as small amounts of uncertainty in the permeability of geological formations, appears to impact prediction uncertainty far more than the small amount of uncertainty introduced from the model abstraction step.

It is concluded that estimating effective pore expansivity and pore compressibility coefficients (a) from high-fidelity THM models, or (b) directly from site characterisation data (preferred) is an acceptable THM-to-TH abstraction approach. Uncertainties in the predicted maximum overpressures caused by uncertainties in the estimated, effective pore expansivity and pore compressibility coefficients are acceptable; the influence of residual errors from the model abstraction process on predictions of interest (e.g., maximum overpressures) is considerably smaller than the influence of random and systematic errors caused by the uncertainties on other parameters and model assumptions.

A variety of topics would benefit from additional studies in the in future, for example:

- Resolve the remaining inconsistencies that exist between the Code_Aster and iTOUGH2 models, such as simulated maximum pressures, near-tunnel properties (e.g., pressure in the EDZ at P12), nearfield properties (saturation and pressures within the tunnel), change in porosity (i.e., function of change in capillary pressure and saturation), and potential differences related to relative permeability and capillary pressure functions.
- Optimize the model calibration technique to improve the inverse solution and reduce uncertainty in the predictions of interest (e.g., perform data worth analysis to help select new calibration data that minimize uncertainty in predicted maximum pressures)
- In-depth study of differences in handling of bentonite properties between iTOUGH and Code_Aster models

9 References

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App. A Code_Aster: 2D HLW model implementation

A.1 Methods

A.1.1 Model setup

The assessment of repository induced effects in the nearfield of SF/HLW repository requires the modeling of non-isothermal hydro-mechanical phenomena. For this, a coupled two-phase flow and mechanical numerical model is developed using the THHM module of Code_Aster (EDF 2024). The numerical model described here follows the hydrogeological setting implemented in the on-going SF/HLW tunnel component modelling activity in the context of the gas synthesis report.

The numerical model presented here is a 2-D plain-strain finite element model, representing the stack of geological formations at the location of the SF/HLW component model in Nördlich Lägern. The model comprises the 22 sequences of Mesozoic formations from the Permocarbon to the Malm, as shown in Fig. A-1. Only half of the tunnel drift is considered due to the symmetry. The distance between the axes of two adjacent tunnels is 40 m. Therefore, the geometry has been chosen to consist of a rectangle of half of that distance, i.e., 20 m width, representing a vertical section from the top surface to the Permocarbon formation across half of an excavated tunnel. The center of the excavation is located on the left boundary of the model, and the emplacement tunnel is in the middle of the host rock layer “Opalinus Clay” (OPA) at a burial depth of 910 m. The tunnel has a radius of 1.925 m. The excavation is filled with a canister of 0.525 m radius sitting on bentonite pedestal of 0.4 m half-width; the rest of the excavation is filled with bentonite buffer. After the excavation, a 0.5 m-thick liner is emplaced and a zone of excavated damage zone (EDZ) is explicitly defined (outer radius: 3.255 m). The model mesh discretizes the tunnel as a semicircular cavity with a finer mesh that converges to a coarser mesh away from the tunnel.

Regarding boundary conditions, horizontal displacement is fixed on the left boundary. Because of the repetition of the problem (multiple tunnels), the horizontal displacement is also fixed on the right boundary. Vertical displacement is prevented on the bottom boundary of the model. Body forces (gravity) are applied on the entire model, meaning that stresses and water pressures vary with depth. Pore water pressure is fixed at hydrostatic values on the top and bottom of the model, and no flow conditions apply to both vertical model boundaries. An initial temperature gradient of 0.043 °C/m is assumed with a 10 °C offset corresponding to the near-surface ground water temperature. Gas pressure is fixed to the atmospheric pressure of 1.0E5 Pa to the entire model throughout the simulations.

The initial equilibrium is obtained by applying hydrostatic pore water pressure and the dead load on the entire medium with an isotropic stress state for one million years. The model directly considers gravity and the initial stress field that is assumed to be a geostatic linear distribution of stresses and pore pressures. The values are calculated analytically and attributed to the Gauss points of each element.

The simulations consider three phases: (i) an initialization phase that lasts 1 million years in order to establish an equilibrated pressure, temperature and stress field through the entire model; (ii) a ventilation phase of 2 years assuming liner installation at the beginning and ventilating the tunnel with a relative humidity of 60 %, a temperature of 28 °C and atmospheric pressure inside the tunnel; and (iii) a post-closure phase up to 100,000 years assuming emplacement of the canister and the bentonite backfill including heat generation of the canister. The current model does not include gas generation in the post-closure phase but assumes gas with the properties of hydrogen for the

ventilation phase. Note that the THM simulation of Code_Aster requires a short (10 days) excavation phase, in which the capillary pressure and the nodal forces at the tunnel wall are assumed to drop to 0 to mimic the approaching excavation front.

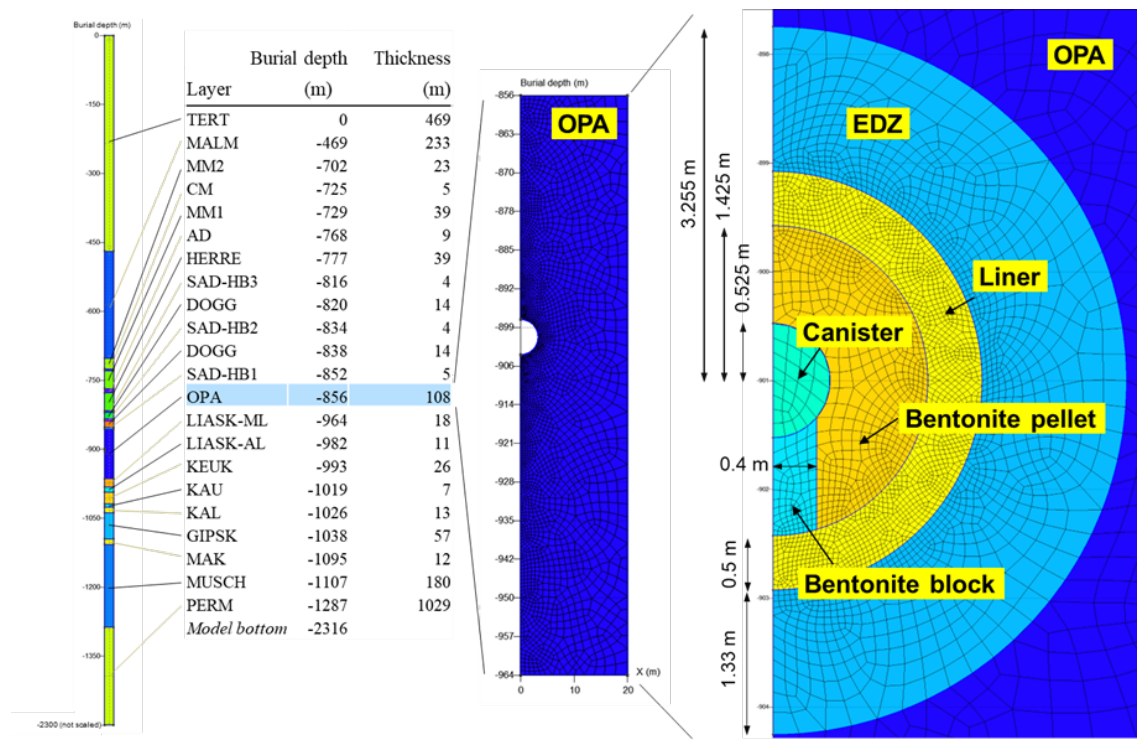


Fig. A-1: Stratigraphic layers in the SF/HLW model for NL and dimensions of carved elements

A.1.2 Model parameters

The parameters used for the Code_Aster modeling are listed in Tab. A-1.

Tab. A-1: Reference points used for the evaluation of Code_Aster and iTOUGH2 results

Layer ID	Por [-]	k _{xyz} [m ²]	E [Pa]	v [-]	c _p ¹ [Pa ⁻¹]	Rho [kg/m ³]	Exp [Pa ⁻¹]	Spht [J/kg/°C]	Cwet [W/m/°C]	Cdry [W/m/°C]	VG_N [-]	VG_P0 ² [Pa]	Slrk ³ [-]
TERT	0.09	1.00E-16	1.15E+10	0.27	1.67E-09	2,700	1.70E-05	995	4.267	4.267	1.67	1.45E+05	0.5
MALM	0.09	9.08E-17	1.15E+10	0.27	1.67E-09	2,700	1.70E-05	995	2.735	2.735	1.67	1.52E+05	0.5
MM2	0.063	1.82E-20	1.15E+10	0.27	2.38E-09	2,707	1.70E-05	995	2.735	2.735	1.67	1.08E+07	0.5
CM	0.03	9.08E-20	1.15E+10	0.27	5.00E-09	2,706	1.70E-05	995	2.735	2.735	1.67	4.81E+06	0.5
MM1	0.074	1.82E-20	1.15E+10	0.27	2.03E-09	2,708	1.70E-05	995	2.735	2.735	1.67	1.08E+07	0.5
AD	0.12	1.82E-21	2.30E+10	0.27	1.25E-09	2,708	1.70E-05	995	2.735	2.735	1.67	3.40E+07	0.5
HERRE	0.026	9.08E-20	1.15E+10	0.27	5.77E-09	2,704	1.70E-05	995	2.735	2.735	1.67	4.81E+06	0.5
SAD-HB3	0.123	2.22E-21	8.00E+09	0.27	1.22E-09	2,715	1.70E-05	995.5	2.527	2.527	1.67	3.08E+07	0.5
DOGG	0.123	2.22E-21	8.00E+09	0.27	1.22E-09	2,715	1.70E-05	995.5	2.527	2.527	1.67	3.08E+07	0.5
SAD-HB2	0.123	2.22E-21	8.00E+09	0.27	1.22E-09	2,715	1.70E-05	995.5	2.527	2.527	1.67	3.08E+07	0.5
DOGG	0.123	2.22E-21	8.00E+09	0.27	1.22E-09	2,715	1.70E-05	995.5	2.527	2.527	1.67	3.08E+07	0.5
SAD-HB1	0.123	2.22E-21	8.00E+09	0.27	1.22E-09	2,715	1.70E-05	995.5	2.527	2.527	1.67	3.08E+07	0.5
OPA	0.115	9.08E-22	7.00E+09	0.27	2.10E-09	2,700	1.70E-05	995	2.1	1.4	1.67	4.81E+07	0.5
LIASK-ML	0.075	4.54E-21	1.15E+10	0.27	2.00E-09	2,689	1.70E-05	995	1.98	1.98	1.67	2.15E+07	0.5
LIASK-AL	0.083	1.82E-21	1.15E+10	0.27	1.81E-09	2,684	1.70E-05	995	1.98	1.98	1.67	3.40E+07	0.5
KEUK	0.108	2.06E-21	1.15E+10	0.32	1.39E-09	2,774	1.70E-05	995	1.98	1.98	1.67	3.19E+07	0.5
KAU	0.087	7.43E-21	1.15E+10	0.27	1.73E-09	2,799	1.70E-05	995	1.98	1.98	1.67	1.68E+07	0.5
KAL	0.121	9.08E-15	1.15E+10	0.27	1.24E-09	2,810	1.70E-05	995	1.98	1.98	1.67	1.52E+04	0.5
GIPSK	0.091	9.08E-21	2.80E+09	0.27	1.65E-09	2,808	1.70E-05	995	1.98	1.98	1.67	1.52E+07	0.5
MAK	0.017	9.08E-21	1.15E+10	0.27	9.00E-09	2,920	1.70E-05	995	6.263	6.263	1.67	1.52E+07	0.5
MUSCH	0.12	4.54E-14	1.15E+10	0.27	1.25E-09	2,700	1.70E-05	995	6.263	6.263	1.67	6.81E+03	0.5
PERM	0.12	1.00E-18	1.15E+10	0.27	1.25E-09	2,700	1.70E-05	995	2.58	2.58	1.67	1.45E+06	0.5

Tab. A-1: Cont.

Layer ID	Por [-]	k _{xyz} [m ²]	E [Pa]	v [-]	c _p ¹ [Pa ⁻¹]	Rho [kg/m ³]	Exp [Pa ⁻¹]	Spht [J/kg/°C]	Cwet [W/m/°C]	Cdry [W/m/°C]	VG_N [-]	VG_P0 ² [Pa]	Slrk ³ [-]
EDZ	0.115	9.08E-21	2.70E+09	0.27	1.70E-09	2,700	1.70E-05	995	1.7	1.4	1.6	1.08E+07	0.5
LINER	0.1	1.00E-18	2.00E+10	0.27	7.00E-10	2,650	1.50E-05	905.5	2.3	1.4	2	2.00E+06	0.05
CANIS	0.001	1.00E-20	2.10E+11	0.29	0	7,850	1.20E-05	440	52.5	52.5	1.42	2.19E+07	0
BLOCK	0.33	2.50E-21	3.00E+08	0.2	3.00E-09	2,699	2.50E-05	1,058	1.3	0.35	1.42	2.19E+07	0
PELLET	0.33	3.50E-20	1.86E+08	0.2	3.00E-09	2,699	2.50E-05	893	1.3	0.35	1.67	1.00E+07	0

¹ Pore compressibility values are used for TH simulations only. Note that they are not derived from E and v but originate from a different data set.

² VG_Sr is set to 0.01 for all domains.

³ Sgr is set to 0 for all domains.

A.1.3 Stress path analysis

The THM simulation results of Code_Aster are used to calculate the stress evolution. The stress path is illustrated in the p-q diagram, where p is the mean effective stress and q is the deviator stress. For triaxial conditions, they can be written in 2D as

$$q = S1' - S3' \quad (A9-1)$$

$$p' = \frac{(S1' + 2 \cdot S3')}{3} \quad (A9-2)$$

and in 3D as

$$q = \sqrt{\frac{(S1' - S3')^2 + (S1' - S2')^2 + (S2' - S3')^2}{2}} \quad (A9-3)$$

$$p' = \frac{(S1' + S2' + S3')}{3} \quad (A9-4)$$

where S1', S2', and S3' are the effective principal stresses.

The failure line is written as

$$q_f = m \cdot \left(p + \frac{c}{\tan \varphi} \right) \quad (A9-5)$$

where c is the cohesion, φ is the angle of internal friction, and

$$m = \frac{6 \sin \varphi}{3 - \sin \varphi} \quad (A9-6)$$

Since iTOUGH2 does not provide any stress values, the stress path can be roughly approximated by calculating the effective stress (S1', S2' or S3') as

$$\sigma' = \sigma_{ini} - \Delta P + \Delta \sigma_T \quad (A9-7)$$

where σ_{ini} is the total initial stress (S1, S2 or S3), ΔP is the pressure change, and $\Delta \sigma_T$ the change in total stress due to temperature changes (ΔT) that can be written as

$$\Delta \sigma_T = \frac{3E\alpha_s\Delta T}{1-2\nu} \quad (A9-8)$$

where E is the Young's modulus, α_s is thermal expansion coefficient, and ν is Poisson's ratio. The thermal stress component assumes constant volume of the bulk material.

In addition to the stress path, results are displayed in terms of the slip tendency. Here, the slip tendency is simply defined as

$$s = \frac{q}{q_f} \quad (\text{A9-9})$$

In words, this means that the slip tendency is the ratio of the deviator stress and the deviator stress at the failure line for the same mean effective stress, i.e., it is a measure of how critically stressed the rock or backfill material is. A slip tendency value of one or larger results in failure.

A.2 Modeling results

The Code_Aster model was used to simulate two base cases: (i) a fully coupled thermo-hydro-mechanical (THM) simulation and (ii) a thermo-hydraulically (TH) coupled simulation. This section first describes the reference points used to evaluate the time-series of the simulations. Then, the THM results are described. Lastly, the TH results are compared to the THM results.

A.2.1 Reference points

For the evaluation and comparison of Code_Aster and iTOUGH2 results, a set of reference points in the tunnel and host rock were defined (Fig. A-2 and Tab. A-2).

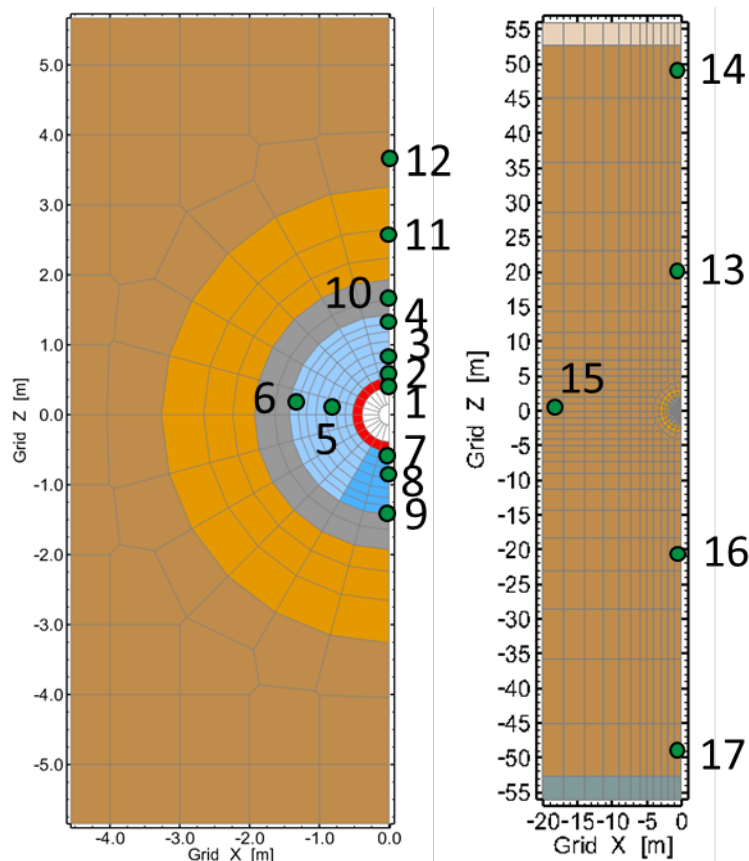


Fig. A-2: Sketch of reference points used for the evaluation of Code_Aster and iTOUGH2 results

Tab. A-2: List of reference points used for the evaluation of Code_Aster and iTOUGH2 results

Point	Description
P1	Canister top
P2	Pellets right above canister
P3	Pellets 0.8 m above center of canister
P4	Pellets 1.3 m above center of canister
P5	Pellets 0.8 m lateral
P6	Pellets 1.3 m lateral
P7	Blocks right below canister
P8	Blocks 0.8 m below center of canister
P9	Blocks 1.3 m below center of canister
P10	Liner 1.7 m above center of canister
P11	EDZ 2.6 m above center of canister
P12	Opalinus Clay right above EDZ
P13	Opalinus Clay 20 m above center of canister
P14	Opalinus Clay 50 m above center of canister
P15	Opalinus Clay 20 m lateral
P16	Opalinus Clay 20 m below center of canister
P17	Opalinus Clay 50 m below center of canister

A.2.2 THM results

Fig. A-3 to Fig. A-5 show the spatial distributions of pressure, water saturation and temperature in the HLW nearfield during the early-emplacement between 5 and 170 years for the THM case. Fig. A-3a to Fig. A-5a show the spatial distributions of pressure, water saturation and temperature in the OPA after 10, 50, 100 and 170 years for the THM case, whereas Fig. A-3b to Fig. A-5b depict the zoom into the nearfield of canister after 5, 10, 20 and 50 years. The temperature increase due to the heat generation in the HLW canister leads to build-up of pressure in the host rock around the HLW tunnel, whereas the pressures in the tunnel remain at values close to atmospheric conditions due to the ventilation phase that occurred before. The water saturation levels are at lower values and suction remains in the backfill materials of the tunnels, but the host rock is fully saturated with water. Fig. A-4b shows that the water saturation front moves upward in the bentonite pedestal and inward in the bentonite buffer.

Fig. A-6 to Fig. A-9 show the temporal evolution of pressure, water saturation, temperature and porosity up to 100,000 years at selected reference points. Maximum pressures of about ca. 16 MPa are reached in the Opalinus Clay at 20 m lateral distance from the HLW tunnel. Pressures in the tunnel are at atmospheric conditions until about 300 years, then the pressure starts to increase. This corresponds to the time when these reference points resaturate with water. The temperature peak is highest in the canister and then gradually decreases with increasing distance from the

canister. A maximum temperature of about 120 °C is reached at the canister. Porosity changes are largest in the bentonite because pressure changes from a regime of high suction to fully saturated conditions whereas changes in the EDZ and host rock are much smaller.

Fig. A-10 illustrates the stress path (p-q plot in 3D) of two reference points (P13 and P15) in the Opalinus Clay using a failure criterion at a friction angle of 20° and a cohesion of 1 MPa. The stress remains far away from the failure criterion for P13 (20 m above tunnel) but comes closer to the failure line for P15 (20 m lateral distance of center of tunnel). The stress paths using the thermal stress approximation (see equation A-8-8) remain at the same deviator stress because $\Delta\sigma_T$ is added to all three principal stress components. It can be observed that the stresses using the approximation move closer to the failure line than for the original THM case. Note that the thermal stress approximation is shown here only for demonstration using the pressure and temperature changes from Code_Aster. It shows that this approach could be used together with the iTOUGH2 results to obtain an approximate stress path. The base case simulation was initialized with stress ratios of $k_{0,x}=0.805$ and $k_{0,y}=0.898$, i.e. the vertical stress component is initially the largest one.

Fig. A-11 illustrates the spatial plots of slip tendency for selected times. The point of maximum slip tendency is close to the tunnel at early post-closure times (values above 1 are reached in the host rock adjacent to the tunnel). This point moves laterally outward with increasing time and reaches the right boundary of the model after about 100 years. For a setup with multiple waste tunnels emplaced next to each other, the slip tendency analysis shows that points between the waste tunnels are much more critically stressed than points above and below the tunnels.

The stress path analysis was repeated for two variants using upper and lower bound initial stress states. Fig. A-12 depicts the stress path for initial stress ratios of $k_{0,x}=0.829$ and $k_{0,y}=0.958$. This leads to stress paths that are less critically stressed than for the base case, because initial deviator stresses are lower. The opposed behavior can be observed for the case with lower bound stress ratios with $k_{0,x}=0.773$ and $k_{0,y}=0.811$, which is shown in Fig. A-13. The higher initial deviator stresses lead to stress paths moving closer to the failure line compared to the base case. For the thermal stress approximation in P15, the failure line is reached.

Fig. A-14 presents spatial plots of horizontal and vertical effective stress in the concrete lining at selected times. Over time, horizontal compressive stress (negative values) increases at the top and bottom of the liner, while horizontal tensile stress (positive values) develops along the sides. In contrast, in the vertical direction, compressive stress forms at the sides, whereas tensile stress develops at the top and bottom. Fig. A-15 shows spatial plots of principle stresses. the mean effective stress increases across the concrete lining with time, while the deviatoric stress primarily develops along the inner interface with the bentonite buffer. This is also evident in the slip tendency spatial plots as shown in Fig. A-16, which further illustrate the influence of the material properties of the lining. A lower friction angle and lower cohesion result in a higher slip tendency.

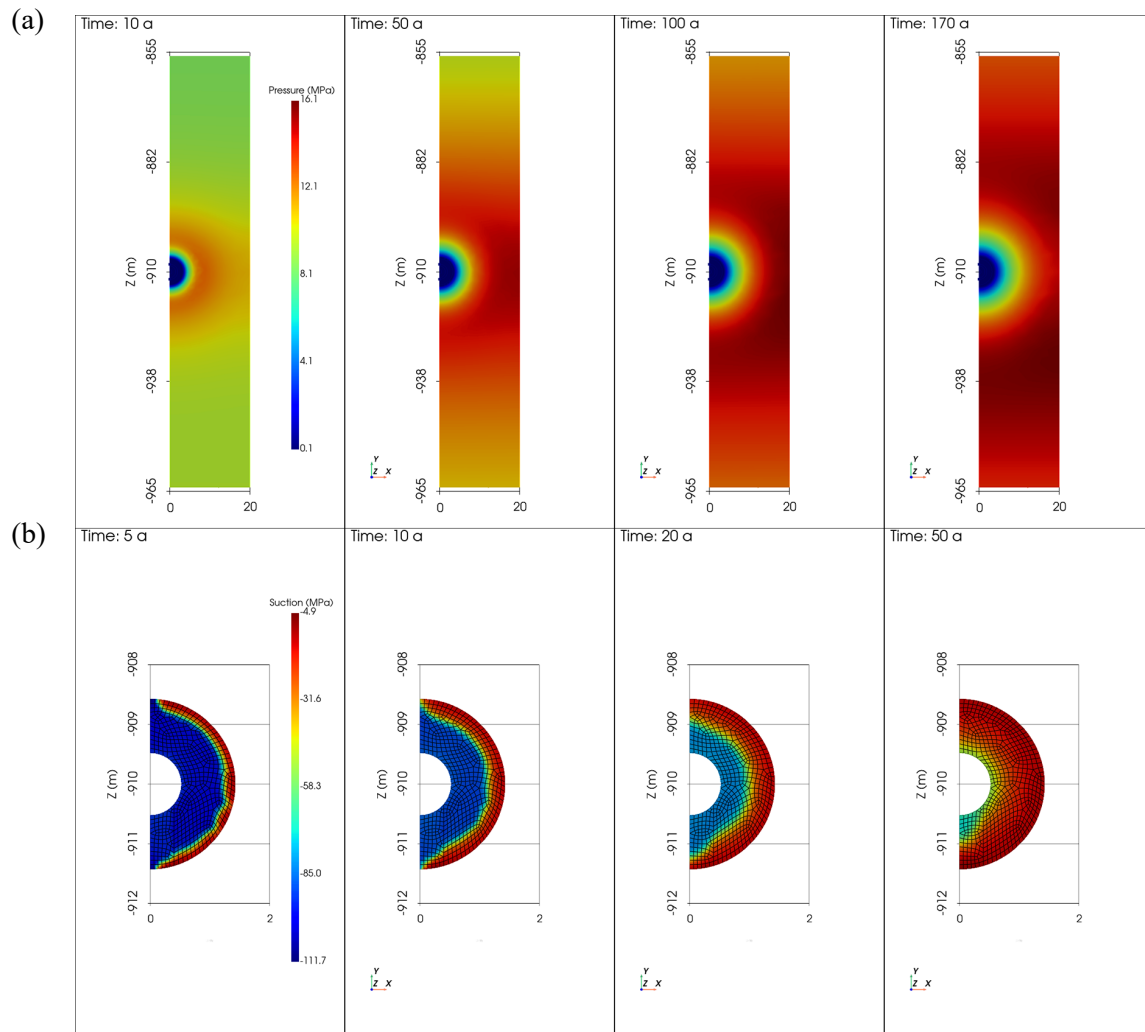


Fig. A-3: Evolution of selected TH state parameters in the HLW nearfield for the THM base case

- (a) Spatial pressure distribution for the first 170 years in the OPA for the THM base case.
 (b) spatial suction distribution for the first 50 years in the bentonite backfill.

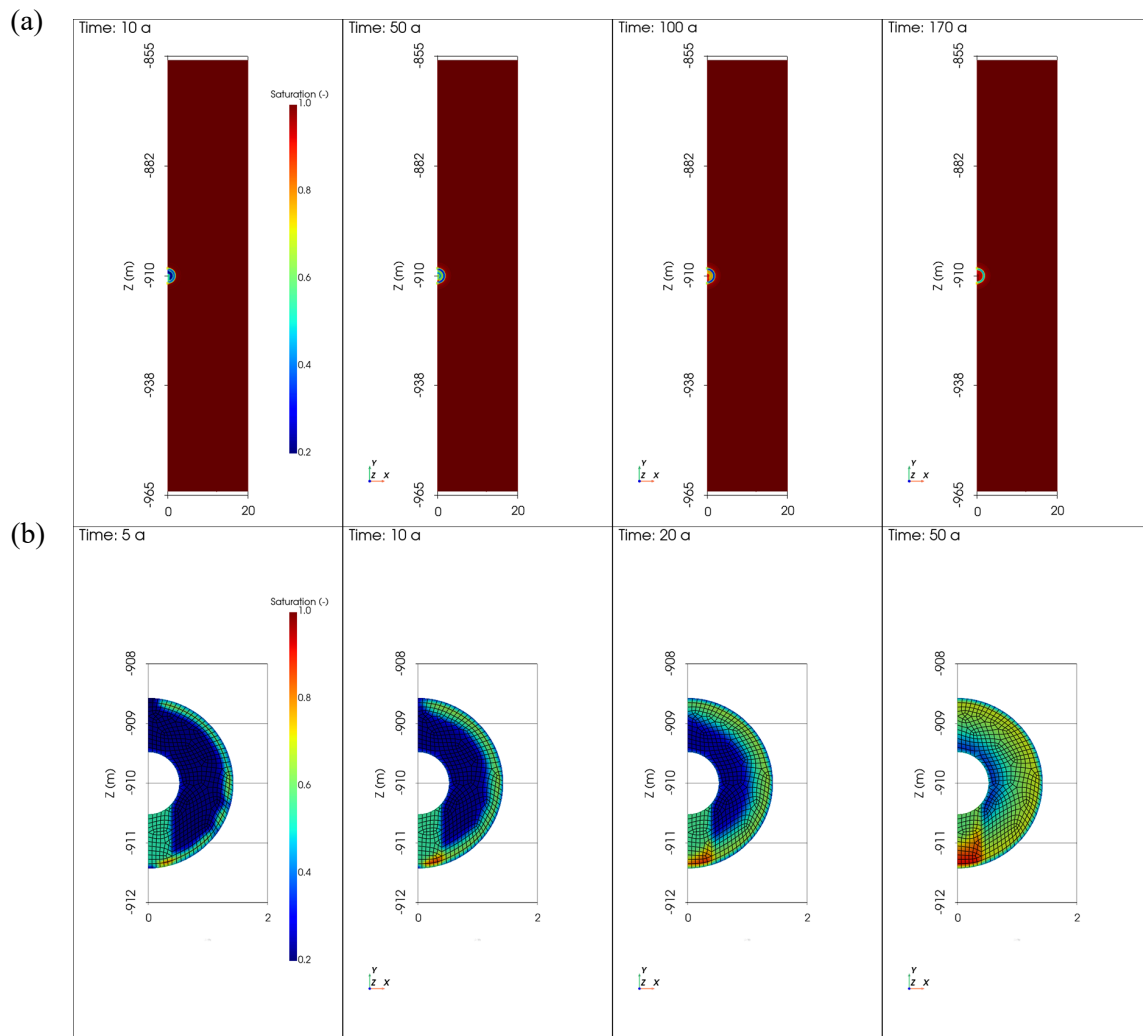


Fig. A-4: Evolution of selected TH state parameters in the HLW nearfield for the THM base case

Spatial water saturation distribution for: (a) the first 170 years in the OPA for the THM base case, and (b) the first 50 years in the bentonite backfill

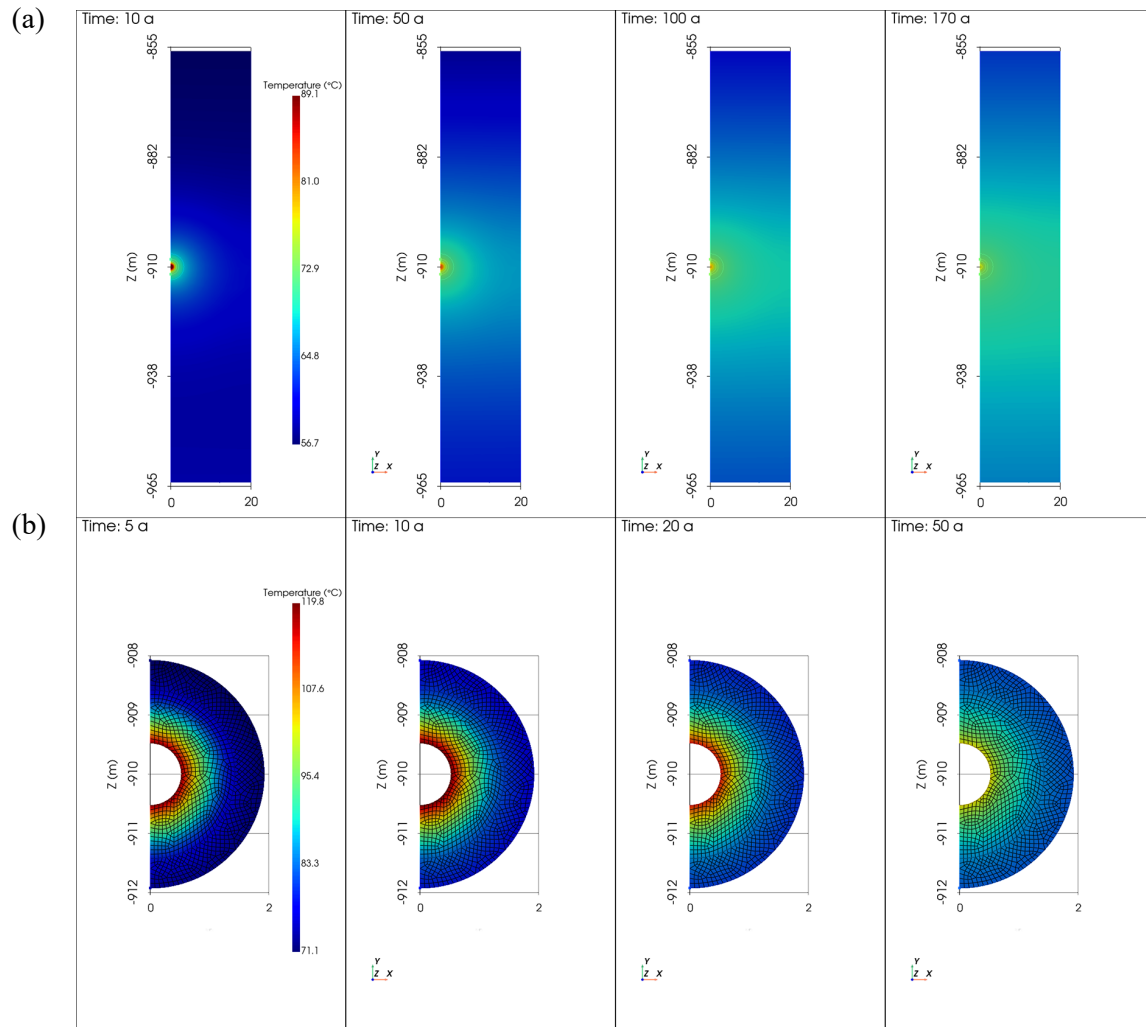


Fig. A-5: Evolution of selected TH state parameters in the HLW nearfield for the THM base case

Spatial temperature distribution for: (a) the first 170 years in the OPA for the THM base case, and (b) the first 50 years in the bentonite backfill

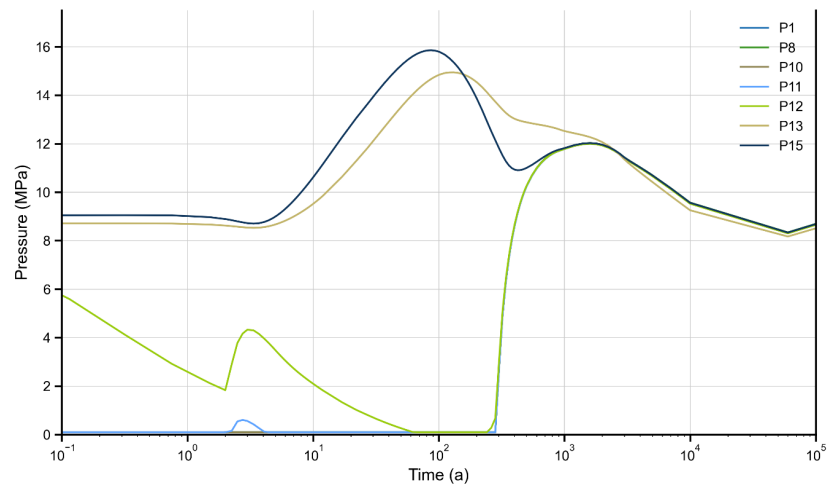


Fig. A-6: Temporal evolution of pressure at selected reference points for the THM base case

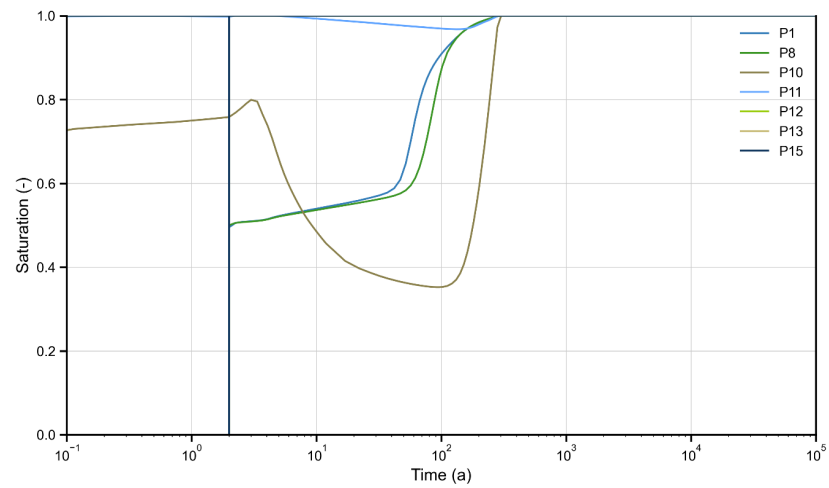


Fig. A-7: Temporal evolution of water saturation at selected reference points for the THM base case

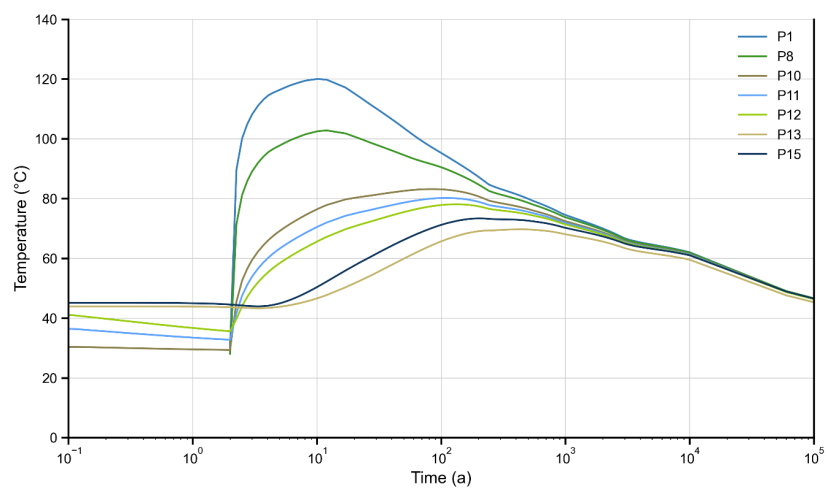


Fig. A-8: Temporal evolution of temperature at selected reference points for the THM base case

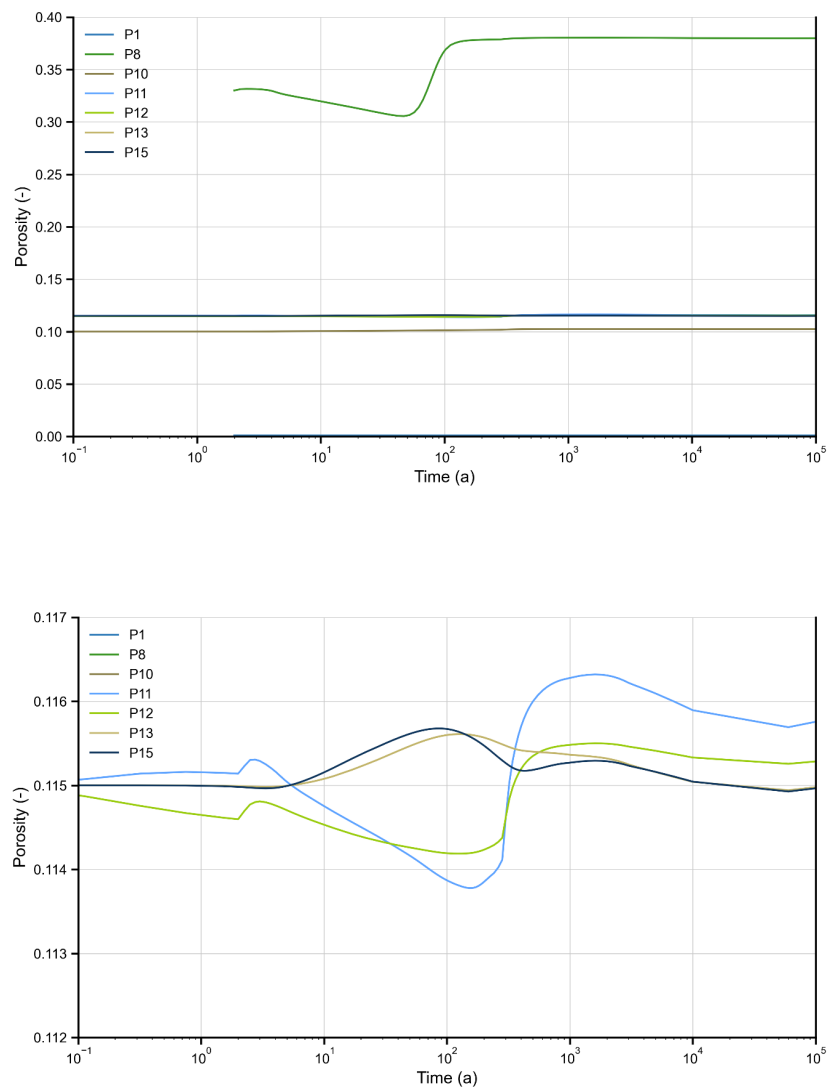


Fig. A-9: Top: temporal evolution of porosity at selected reference points for the THM base case

Bottom: zoom view

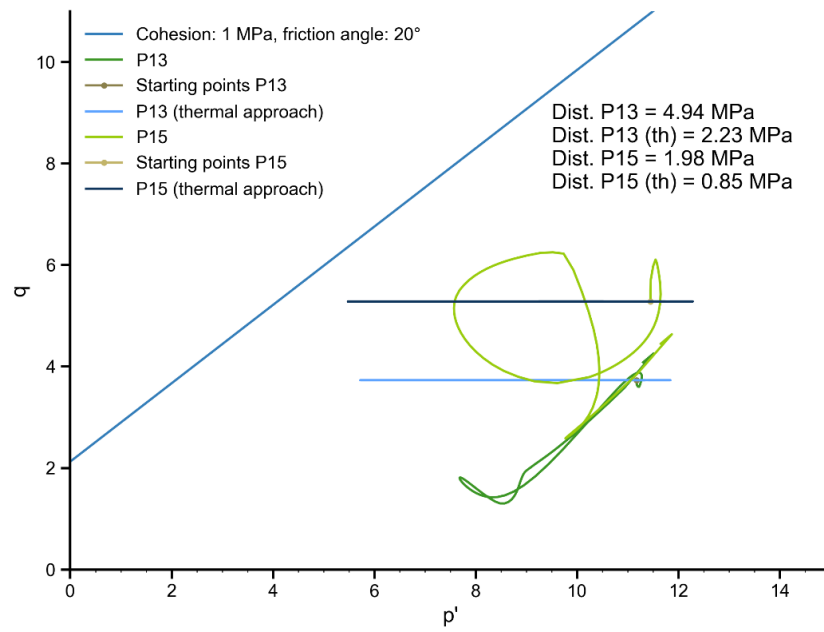


Fig. A-10: Stress path of the THM base case

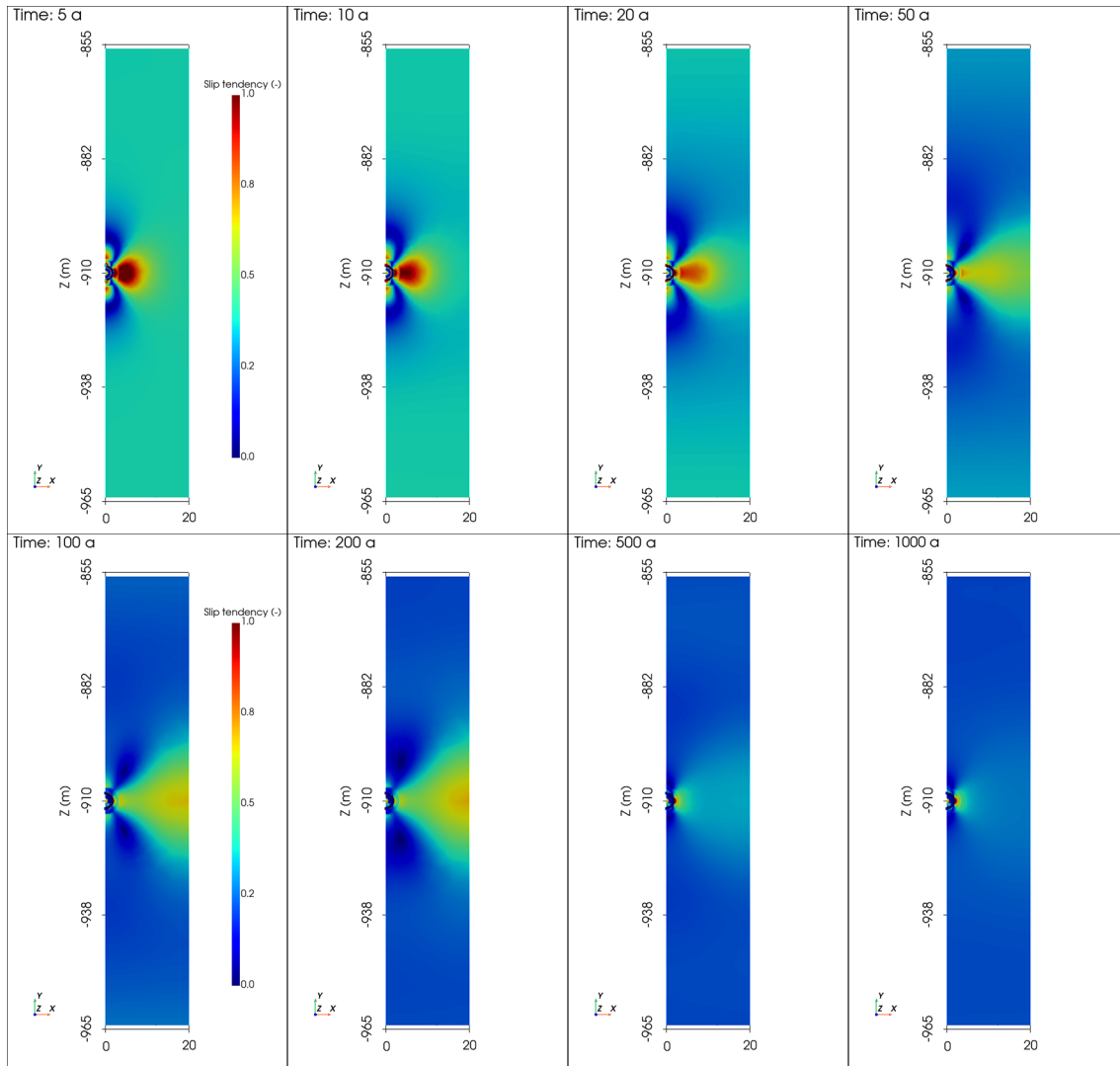


Fig. A-11: Slip tendency for selected times for the THM base case

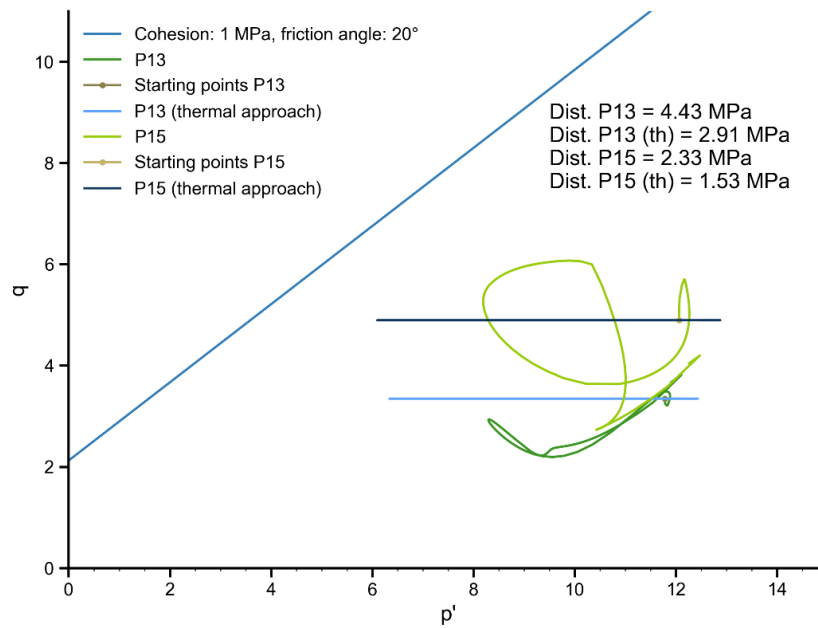


Fig. A-12: Stress path of the THM case with upper bound stress ratios (p-q plot)

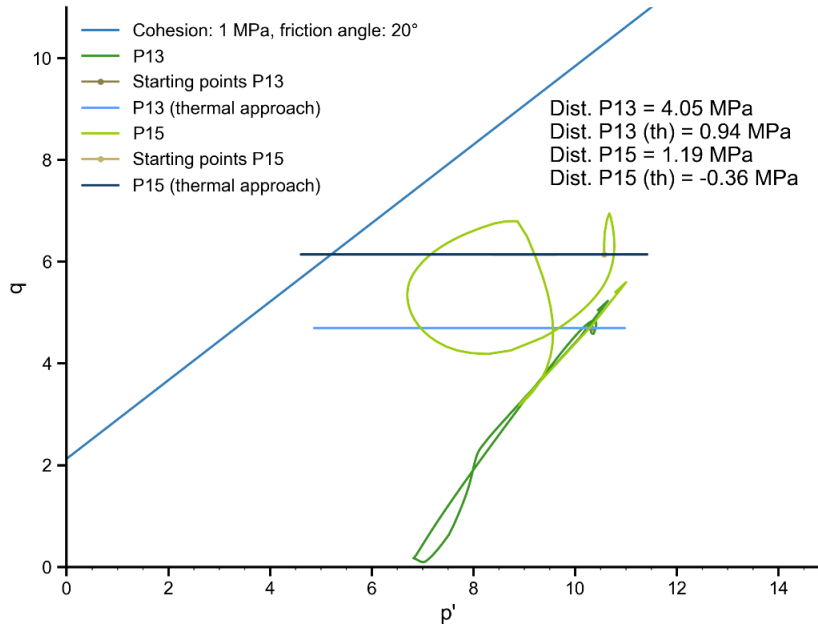


Fig. A-13: Stress path of the THM case with lower bound stress ratios (p-q plot)

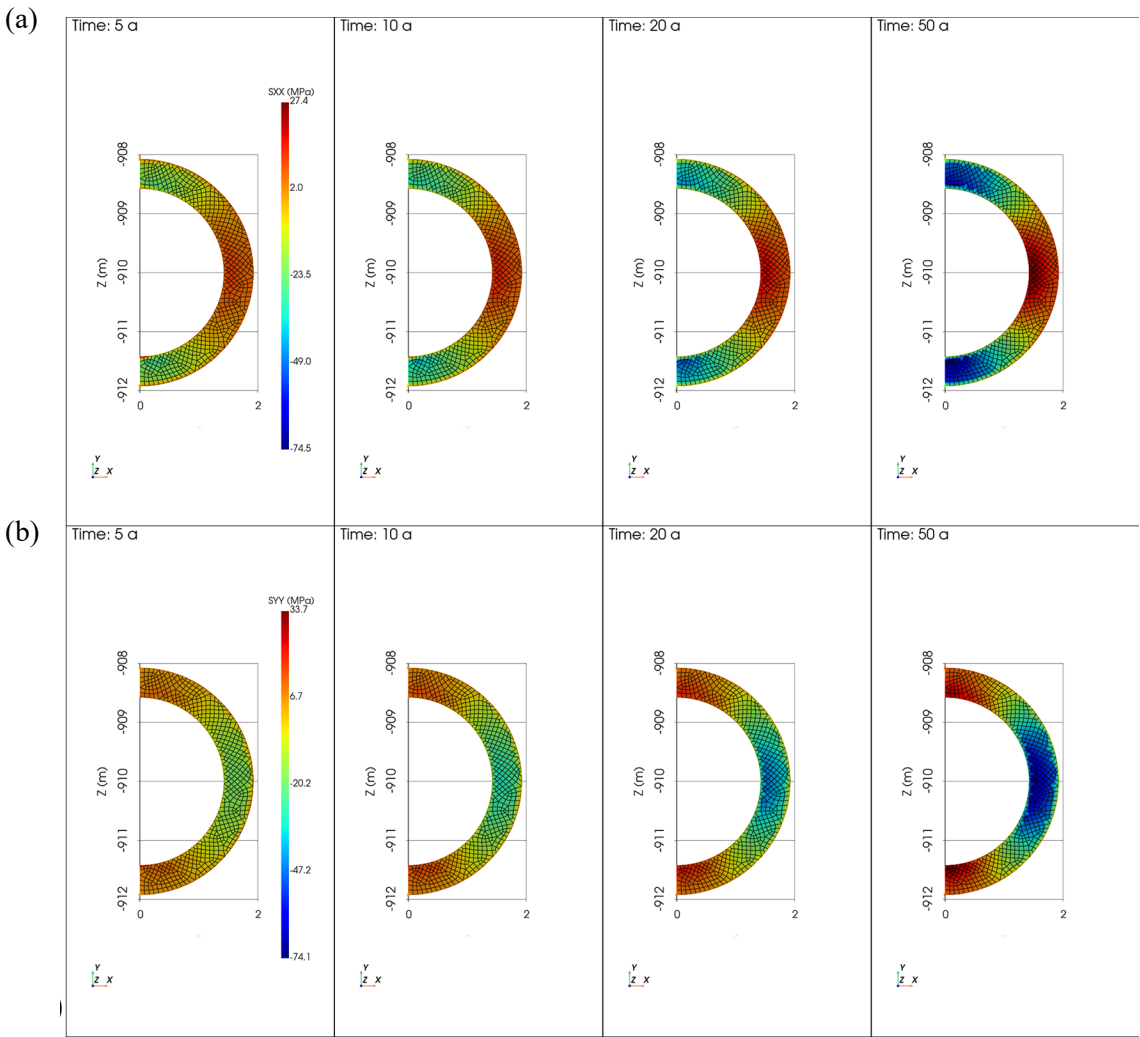


Fig. A-14: Spatial stress distribution for selected times in the concrete lining
(a) horizontal effective stress, (b) vertical effective stress distribution

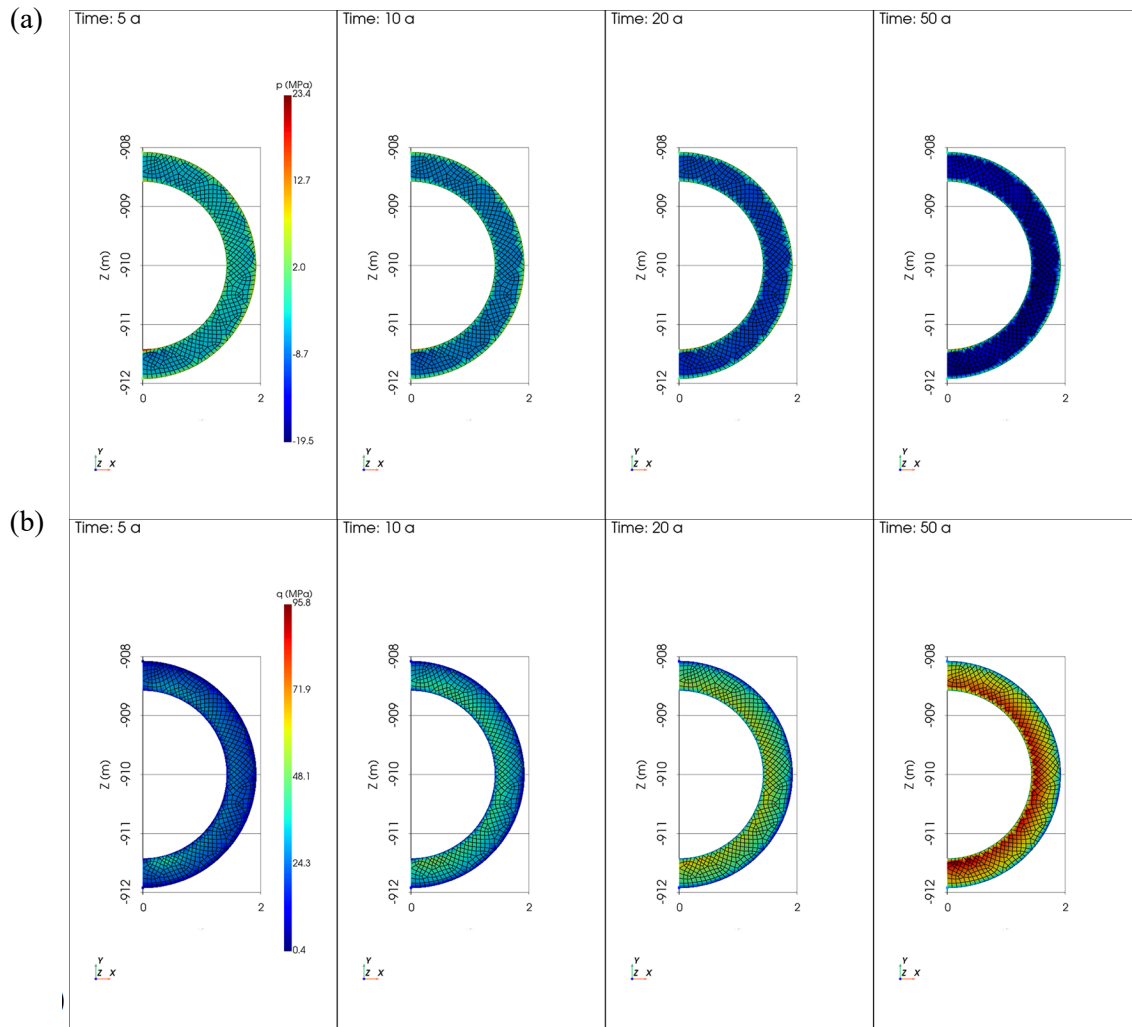


Fig. A-15: Spatial principle stress distribution for selected times in the concrete lining
 (a) mean effective stress p' , (b) deviatoric stress q

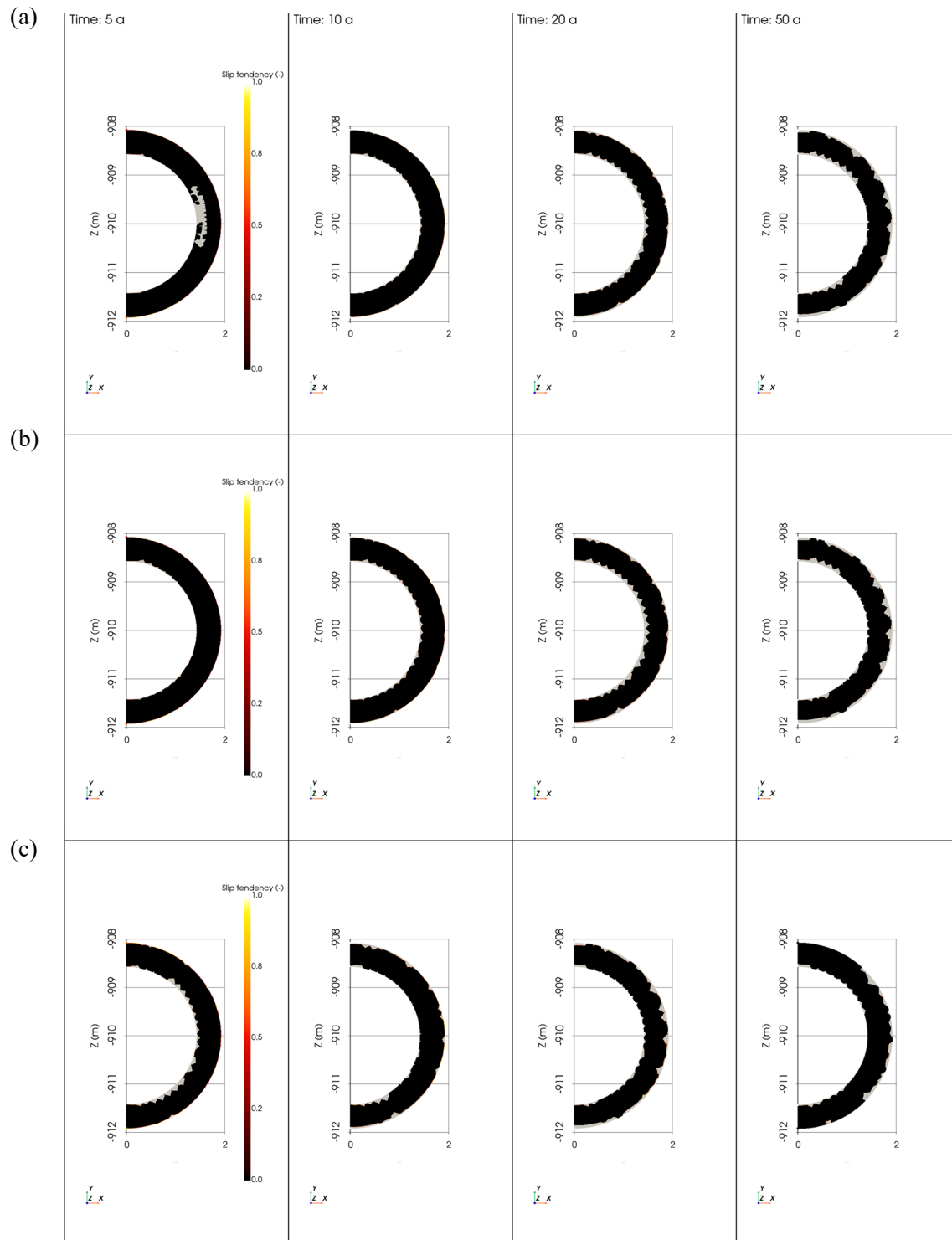


Fig. A-16: Slip tendency for selected times in the concrete lining

(a) $\phi = 15^\circ$ and $c = 1$ MPa (b) $\phi = 20^\circ$ and $c = 1$ MPa, and (c) $\phi = 20^\circ$ and $c = 0$ MPa

A.2.3 TH-THM comparison

Fig. A-18 to Fig. A-20 show the spatial distributions of pressure, water saturation and temperature after 10, 50, 102 and 150 years for the TH case. Like the THM case, pressures are increasing around the tunnel due to the temperature pulse caused by the heat generation from the waste canister. The saturations are also very similar compared to the THM case.

Fig. A-21 to Fig. A-23 illustrate the temporal evolution of pressure, water saturation, temperature and porosity up to 100,000 years for TH case compared to the THM simulation. The pressure in (P11) and right above the EDZ (P12) is significantly lower for TH case. This can be explained by the different setup of the excavation and ventilation phase. In the TH case, the 10-day excavation simulation is absent and therefore, the pressure evolution is different in points close to the tunnel. In regard of the maximum pressures, the TH case shows significantly lower pressures than the THM case. Since the TH case is not constrained by the mechanical framework, the pressure increase is less pronounced than in the THM case. Note that the pore compressibility of the host rock, which is mainly governing the pressure increase due to thermal pressurization, is not the same in the two cases. However, an additional TH test case with a pore compressibility corresponding to the value calculated from the Young's modulus and Poisson's ratio used in the THM simulation still leads to significantly lower maximum pressures in the Opalinus Clay. Hence, the differences seen here can be explained by mechanical effects not considered in TH. The water saturation and temperature time-series of the TH and THM cases are not exactly the same, but overall very similar.

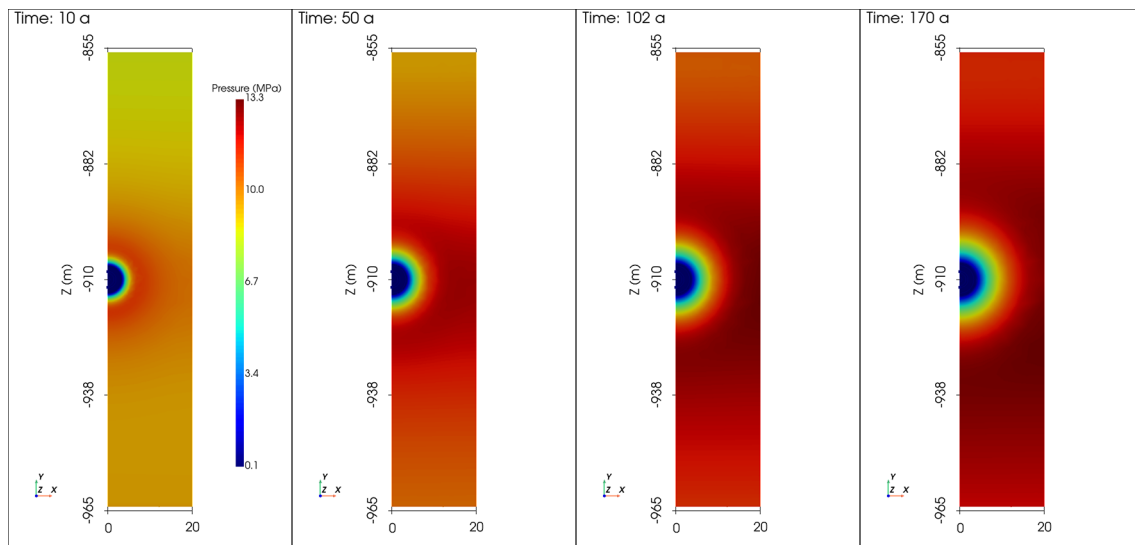


Fig. A-17: Spatial pressure distribution for the first 170 years for the TH case

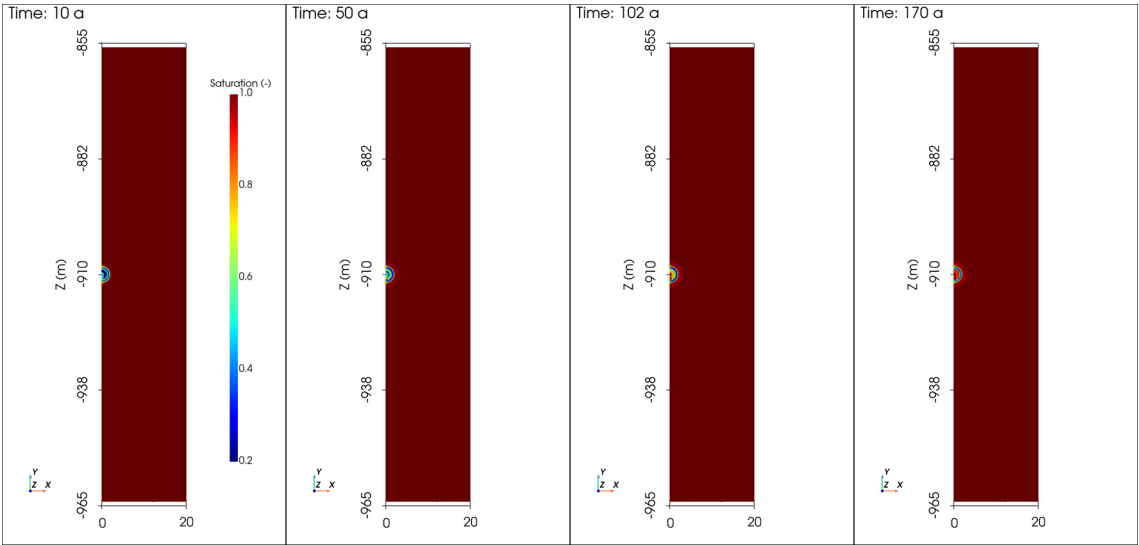


Fig. A-18: Spatial water saturation distribution for the first 170 years for the TH case

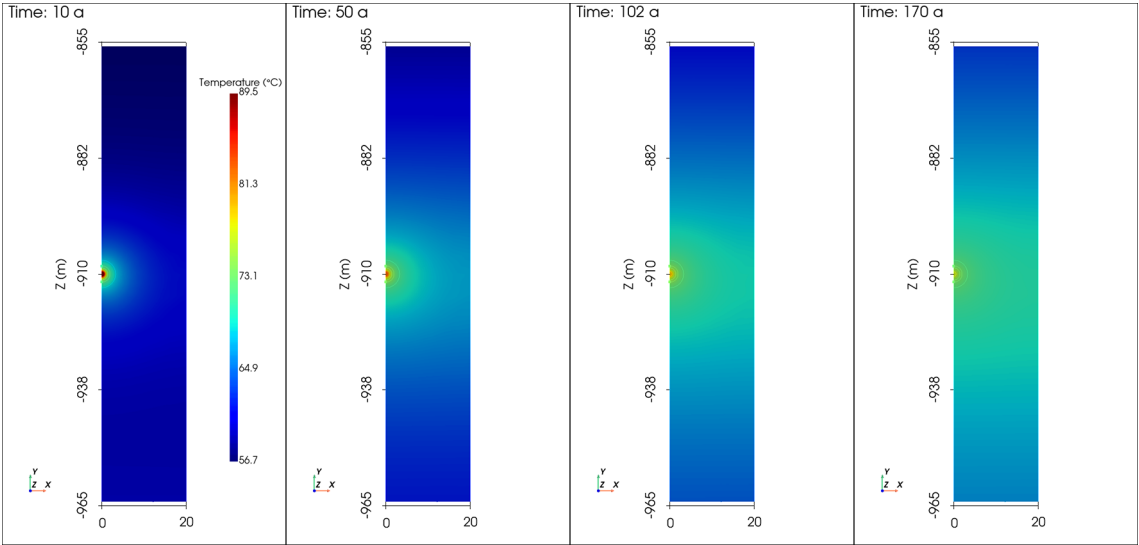


Fig. A-19: Spatial temperature distribution for the first 170 years for the TH case

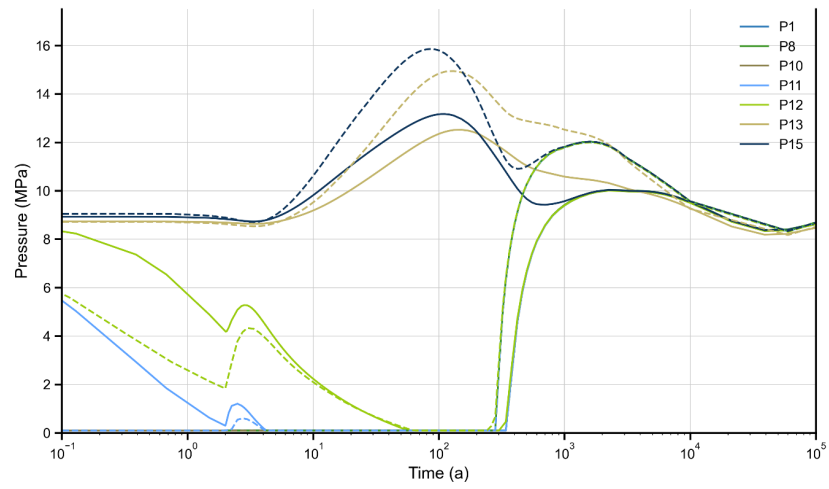


Fig. A-20: Temporal evolution of pressure at selected reference points for the TH case

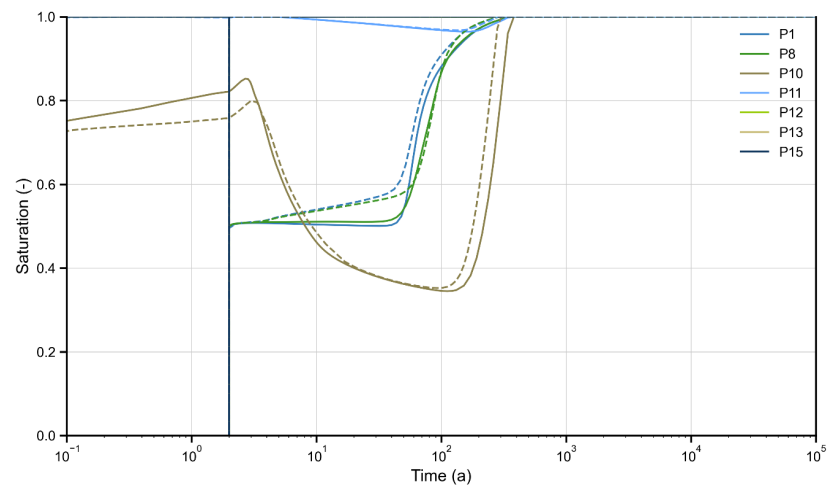


Fig. A-21: Temporal evolution of water saturation at selected reference points for the TH case

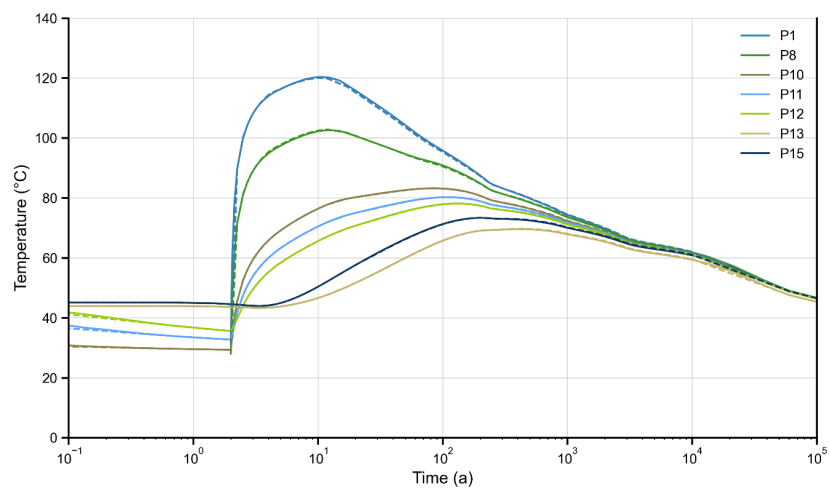


Fig. A-22: Temporal evolution of temperature at selected reference points for the TH case

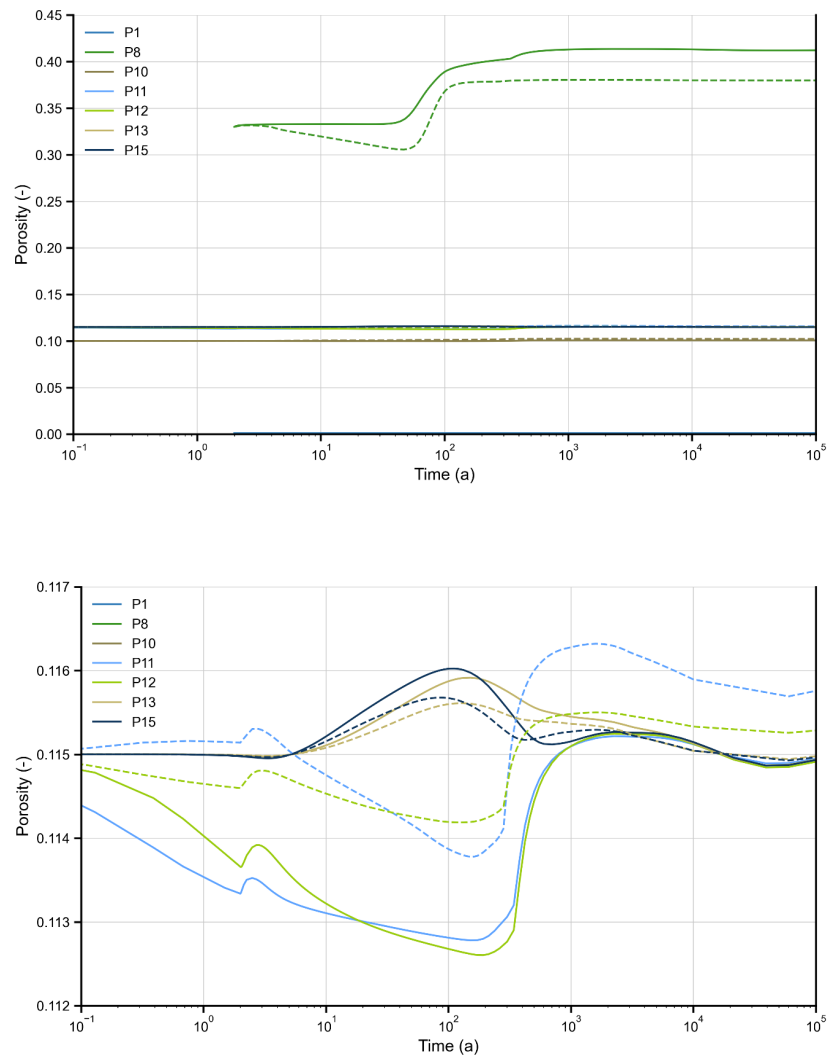


Fig. A-23: Top: temporal evolution of porosity at selected reference points for the TH case
Bottom: zoom view

A.2.4 TH comparison between Code_Aster and iTOUGH2 (Version: March 24)

Fig. A-24 to Fig. A-26 depict the temporal evolution of pressure, water saturation and temperature up to 100,000 years for the TH simulations of Code_Aster and iTOUGH2. Some significant differences in pressure evolution can be seen both in the EDZ and in the Opalinus Clay. In particular, the maximum pressure in the host rock is about 1 MPa higher in iTOUGH2. Significant differences can also be observed in the evolution of the water saturation, especially in the different components of the tunnel. Code_Aster is assuming constant gas pressure at 1 atmospheric pressure throughout the simulation. Therefore, there is no flow in the gas phase. Capillary pressure is a primary variable, while saturation is a secondary variable calculated from the retention curve. On the other hand, iTOUGH2 uses gas pressure and gas saturation as primary variables. Gas pressure can change with time and gas can flow as a separate phase. Capillary pressure is a secondary variable and determined from the gas saturation through the retention curve. The large differences in saturation between the two codes can thus be explained by the basic differences in the setup of the two-phase flow calculations. For the temperature, Code_Aster leads to slightly smaller values than iTOUGH2. Since saturation may also affect the evolution of temperature, the differences in temperature could be explained by the different simulation of the two-phase flow system, as well. However, at the reference points in the host rock farther away from the tunnel, Code_Aster leads to higher temperatures, whereas the pressure increase due to the thermal pressurization is smaller. This counterintuitive observation results from a small residual gas phase (~1 %) established in the host rock for the Code_Aster simulation. Therefore, the fluid in Code_Aster is much more compressible than in iTOUGH2, and the corresponding pressure increase is smaller.

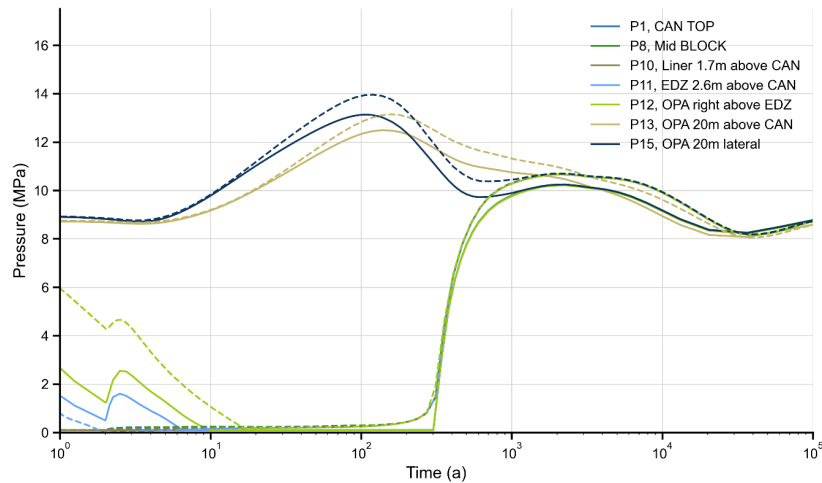


Fig. A-24: Temporal evolution of pressure at selected reference points for the TH case with Code_Aster (solid lines) and iTOUGH2 (dashed lines)

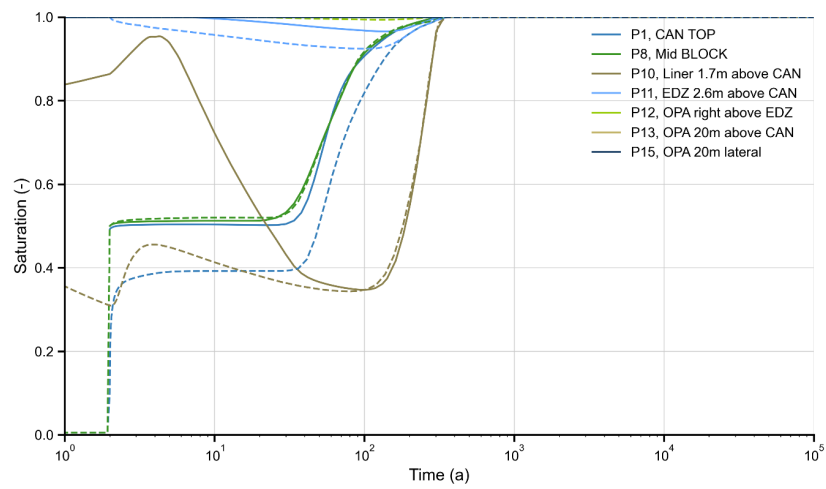


Fig. A-25: Temporal evolution of water saturation at selected reference points for the TH case with Code_Aster (solid lines) and iTOUGH2 (dashed lines)

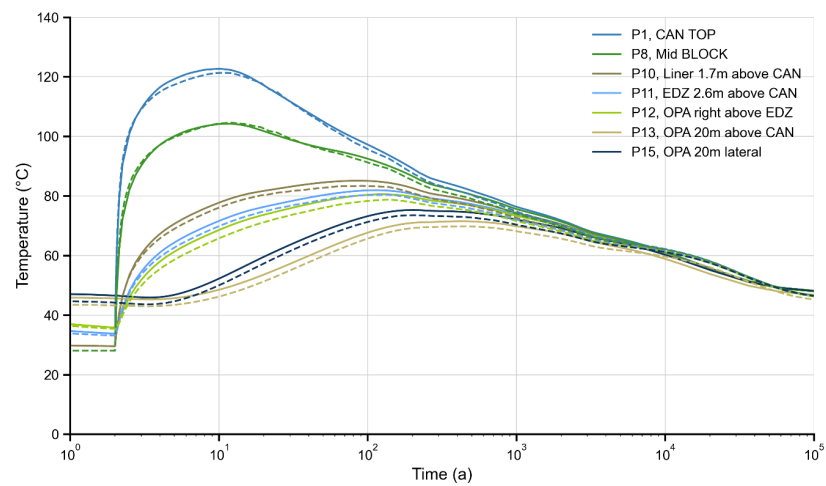


Fig. A-26: Temporal evolution of temperature at selected reference points for the TH case with Code_Aster (solid lines) and iTOUGH2 (dashed lines)

A.2.5 Stress evolution at the canister surface

The evolution of normal stress at the canister surface with time is a key aspect for robust design of the SF canisters. The Code_Aster simulations were utilized to estimate the evolution of normal stresses in a period ranging from the unsaturated phase immediately after canister emplacement up to 100,000 years. Note that a simple elastic model was used for bentonite, based on the assumption that swelling pressure is just proportional to the water pressure development. Negative normal stresses (i.e., tensile stress) in the early post emplacement periods are directly linked to the negative water pressure (capillary pressure in the bentonite), which also results from the assumption of perfect contact between the buffer component and the canister, and it is not the case in reality.

Fig. A-24 to Fig. A-26 depict the temporal evolution of water saturation, porewater pressure and normal stress at the canister surface up to 100,000 years.

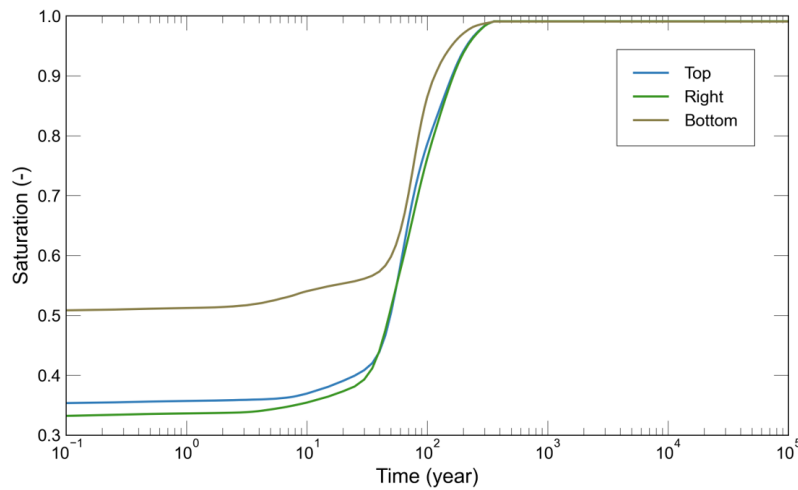


Fig. A-27: Temporal evolution of water saturation at canister surface (top, right and bottom) up to 100,000 years from the THM simulations of Code_Aster

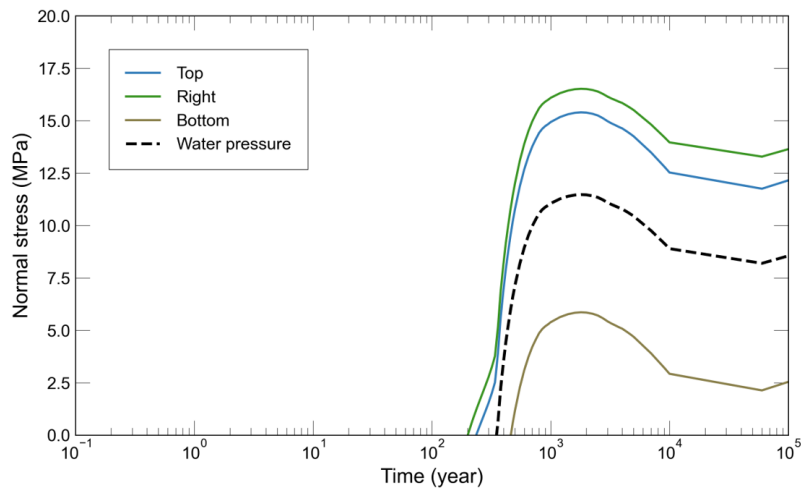


Fig. A-28: Temporal evolution of pore water pressure and of normal stress at canister surface (top, right and bottom) up to 100,000 years from the THM simulations of Code_Aster

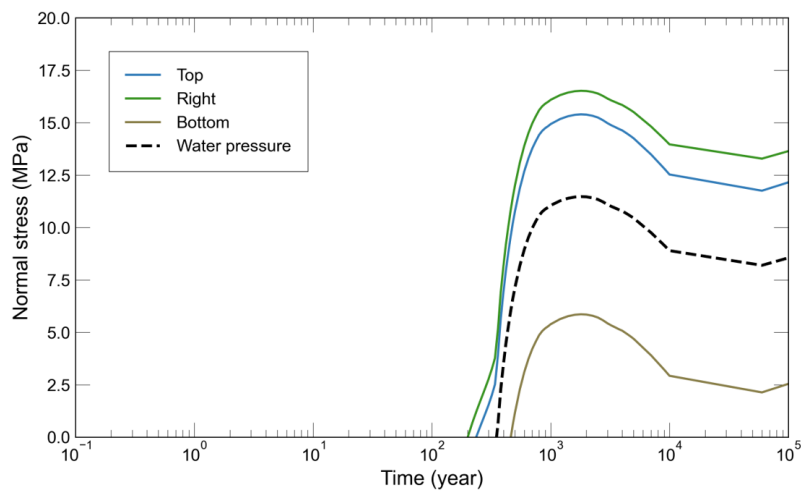


Fig. A-29: Temporal evolution of normal stress at canister surface (top, right and bottom) during the unsaturated phase from the THM simulations of Code_Aster